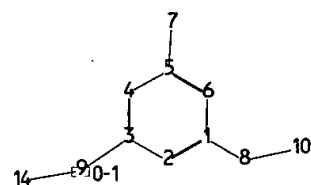
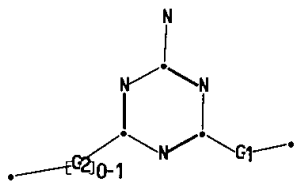


L Number	Hits	Search Text	DB	Time stamp
1	4285	HDL	USPAT; US-PGPUB; EPO; JPO; DERWENT	2002/05/19 10:49
2	1525	HDL adj cholester\$	USPAT; US-PGPUB; EPO; JPO; DERWENT	2002/05/19 10:49
3	1912731	rais\$ or elevat\$	USPAT; US-PGPUB; EPO; JPO; DERWENT	2002/05/19 10:50
4	423	(HDL adj cholester\$) same (rais\$ or elevat\$)	USPAT; US-PGPUB; EPO; JPO; DERWENT	2002/05/19 11:04
5	311	514/245.ccls.	USPAT; US-PGPUB; EPO; JPO; DERWENT	2002/05/19 11:05
6	0	544/213.ccls	USPAT; US-PGPUB; EPO; JPO; DERWENT	2002/05/19 11:06
7	176	544/213.ccls.	USPAT; US-PGPUB; EPO; JPO; DERWENT	2002/05/19 11:06
8	477	514/245.ccls. or 544/213.ccls.	USPAT; US-PGPUB; EPO; JPO; DERWENT	2002/05/19 11:06
9	0	((HDL adj cholester\$) same (rais\$ or elevat\$)) and (514/245.ccls. or 544/213.ccls.)	USPAT; US-PGPUB; EPO; JPO; DERWENT	2002/05/19 11:07
10	52757	triazin\$	USPAT; US-PGPUB; EPO; JPO; DERWENT	2002/05/19 11:07
11	28	((HDL adj cholester\$) same (rais\$ or elevat\$)) and triazin\$	USPAT; US-PGPUB; EPO; JPO; DERWENT	2002/05/19 11:07



chain nodes :

8

ring nodes :

1 2 3 4 5 6

ring/chain nodes :

7 9 10 14

chain bonds :

1-8 3-9 5-7 8-10 9-14

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

1-8 3-9 5-7 8-10 9-14

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G1:O,S,N

G2:C,O

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS

14:CLASS

=>Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=> screen 2016 OR 2026 OR 2039 OR 2040

L1 SCREEN CREATED

=>

Uploading C:\STNEXP4\QUERIES\10005064 (method).str

L2 STRUCTURE UPLOADED

=> que L2 NOT L1

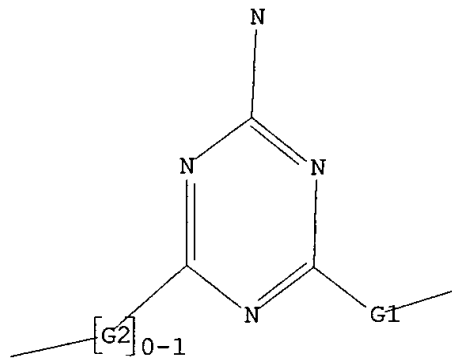
L3 QUE L2 NOT L1

=> d 13

L3 HAS NO ANSWERS

L1 SCR 2016 OR 2026 OR 2039 OR 2040

L2 STR



G1 O,S,N

G2 C,O

Structure attributes must be viewed using STN Express query preparation.

L3 QUE L2 NOT L1

=> s 13 sss sam

SAMPLE SEARCH INITIATED 11:44:16 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 3903 TO ITERATE

25.6% PROCESSED 1000 ITERATIONS

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 74316 TO 81804

PROJECTED ANSWERS: 21441 TO 25551

L4 50 SEA SSS SAM L2 NOT L1

=> s 13 sss ful
FULL SEARCH INITIATED 11:44:23 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 76867 TO ITERATE

100.0% PROCESSED 76867 ITERATIONS 23143 ANSWERS
SEARCH TIME: 00.00.04

L5 23143 SEA SSS FUL L2 NOT L1

=> s 15

L6 6375 L5

=> s hdl cholester?

15172 HDL

140259 CHOLESTER?

L7 6515 HDL CHOLESTER?
 (HDL(W)CHOLESTER?)

=> s 16 (1) 17

L8 0 L6 (L) L7

=> s 16(1)17

L9 0 L6(L)L7

=> s 16(p)17

L10 0 L6(P)L7

=> s 16 and 17

L11 0 L6 AND L7

=> s cholester?

L12 140259 CHOLESTER?

=> s 16 (1) 112

L13 1 L6 (L) L12

=> d 113 bib,ab,hitstr

```
=> s abca? (w) express?
      306 ABCA?
      844177 EXPRESS?
L14      25 ABCA? (W) EXPRESS?
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=> s abca? (p) express?
      306 ABCA?
      844177 EXPRESS?
L15      95 ABCA? (P) EXPRESS?
```

```
=> s l6 and l15
L16      0 L6 AND L15
```

```
=> d his
```

(FILE 'HOME' ENTERED AT 11:42:59 ON 19 MAY 2002)

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FILE 'REGISTRY' ENTERED AT 11:43:04 ON 19 MAY 2002
L1      SCREEN 2016 OR 2026 OR 2039 OR 2040
L2      STRUCTURE UPLOADED
L3      QUE L2 NOT L1
L4      50 S L3 SSS SAM
L5      23143 S L3 SSS FUL
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FILE 'CAPLUS' ENTERED AT 11:44:33 ON 19 MAY 2002
L6      6375 S L5
L7      6515 S HDL CHOLESTER?
L8      0 S L6 (L) L7
L9      0 S L6(L)L7
L10     0 S L6(P)L7
L11     0 S L6 AND L7
L12     140259 S CHOLESTER?
L13     1 S L6 (L) L12
L14     25 S ABCA? (W) EXPRESS?
L15     95 S ABCA? (P) EXPRESS?
L16     0 S L6 AND L15
```

```
=> s coronary arter? or atheroscler?
      44483 CORONARY
      161715 ARTER?
      20291 CORONARY ARTER?
          (CORONARY(W)ARTER?)
      32911 ATHEROSCLER?
L17     50483 CORONARY ARTER? OR ATHEROSCLER?
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=> s l6 and l17
L18     3 L6 AND L17
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=> d l18 1-3 bib,ab,hitstr
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L18 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2002 ACS

AN 2002:90040 CAPLUS

DN 136:135022

TI Preparation of heteroaryl-.beta.-alanine derivatives as antiinflammatory agents and .alpha.4 integrin inhibitors

IN Konradi, Andrei W.; Pleiss, Michael A.; Thorsett, Eugene D.; Ashwell, Susan; Welmaker, Gregory S.; Kreft, Anthony; Sarantakis, Dimitrios; Dressen, Darren B.; Grant, Francine S.; Semko, Christopher; Xu, Ying-Zi

PA Elan Pharmaceuticals, Inc., USA; American Home Products Corporation

SO PCT Int. Appl., 141 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002008222	A2	20020131	WO 2001-US23096	20010720
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK , DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRAI US 2000-220128P P 20000721

OS MARPAT 136:135022

AB Disclosed are a series of heteroaryl-.beta.-alanine derivs. I wherein R is a carboxylic acid; R1 and R2 are independently selected from the group consisting of hydrogen, alkyl, substituted alkyl, alkenyl, substituted alkenyl, cycloalkyl, substituted cycloalkyl, or R1 and R2, together with the nitrogen atom to which they are attached, are joined to form an optionally substituted heterocyclic ring provided that said substituted alkyl, substituted alkenyl and substituted cycloalkyl do not carry an aryl, substituted aryl, heteroaryl or substituted heteroaryl group; Ra and R3 are independently a hydrogen or a Me group; R4 and R5 are independently selected from the group consisting of heteroatom group; n is zero or an integer 1; Alk is a straight or branched alkylene chain; Ar is an optionally substituted arom. or heteroarom. group, as well as their pharmaceutical use as .alpha.4.beta.7 Integrin inhibitors for the treatment of inflammatory diseases. Thus, 3-[4-(3,5-dichloropyrid-4-ylcarboxamido)phenyl]-2-(3-chlorophenylamino)propanoic acid was prepd. as .alpha.4 Integrin inhibitor. The preferred compds. of the invention generally have IC50 values in the .alpha.4.beta.1 and .alpha.a.beta.7 assays of 1 .mu.M and below. In the other assays featuring .alpha. integrins of other subgroups the same compds. had IC50 values of 50 .mu.M and above thus demonstrating the potency and selectivity of their action against .alpha.4 integrins. Title compds. were prepd. for treating an inflammatory condition in a mammalian patient which condition is mediated by Very Late Antigen 4 (VLA-4). Inflammatory condition is selected from the group consisting of asthma, Alzheimer's disease, **atherosclerosis**, AIDS dementia, diabetes, inflammatory bowel disease, multiple sclerosis, rheumatoid arthritis, tissue transplantation, tumor metastasis, meningitis, encephalitis, stroke, nephritis, retinitis, atopic dermatitis, psoriasis, myocardial ischemia and acute leukocyte-mediated lung injury.

IT 263274-37-9P 263274-66-4P 263274-86-8P

not prior art

263274-93-7P 263274-94-8P 263274-95-9P

263274-97-1P 263274-99-3P 263275-01-0P

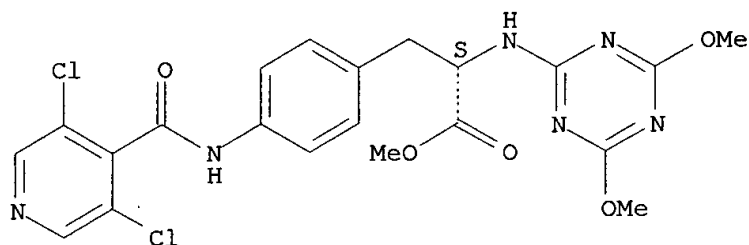
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of heteroaryl-.beta.-alanine derivs. as antiinflammatory agents and .alpha.4 integrin inhibitors)

RN 263274-37-9 CAPLUS

CN L-Phenylalanine, 4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-, methyl ester (9CI) (CA INDEX NAME)

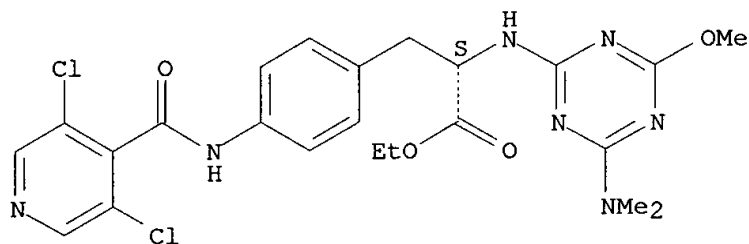
Absolute stereochemistry.



RN 263274-66-4 CAPLUS

CN L-Phenylalanine, 4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[4-(dimethylamino)-6-methoxy-1,3,5-triazin-2-yl]-, ethyl ester (9CI) (CA INDEX NAME)

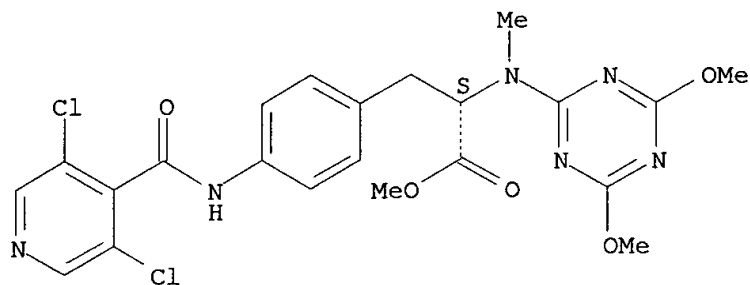
Absolute stereochemistry.



RN 263274-86-8 CAPLUS

CN L-Phenylalanine, 4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-N-methyl-, methyl ester (9CI) (CA INDEX NAME)

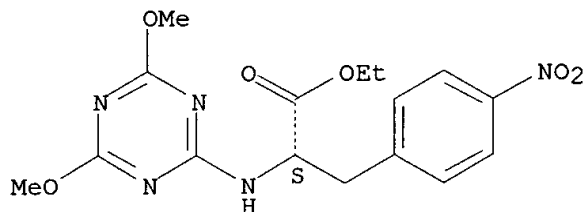
Absolute stereochemistry.



RN 263274-93-7 CAPLUS

CN L-Phenylalanine, N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-nitro-, ethyl ester (9CI) (CA INDEX NAME)

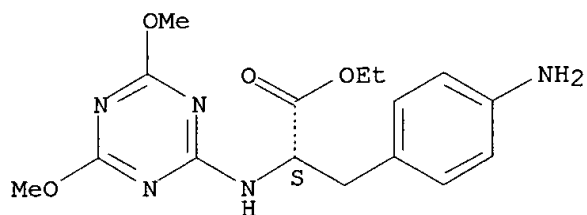
Absolute stereochemistry.



RN 263274-94-8 CAPLUS

CN L-Phenylalanine, 4-amino-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-, ethyl ester (9CI) (CA INDEX NAME)

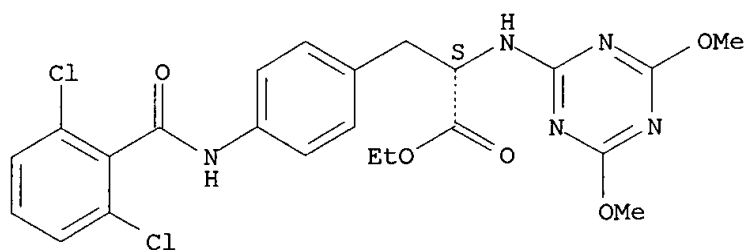
Absolute stereochemistry.



RN 263274-95-9 CAPLUS

CN L-Phenylalanine, 4-[(2,6-dichlorobenzoyl)amino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-, ethyl ester (9CI) (CA INDEX NAME)

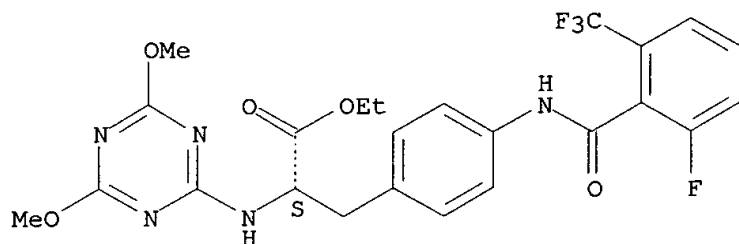
Absolute stereochemistry.



RN 263274-97-1 CAPLUS

CN L-Phenylalanine, N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-[[2-fluoro-6-(trifluoromethyl)benzoyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

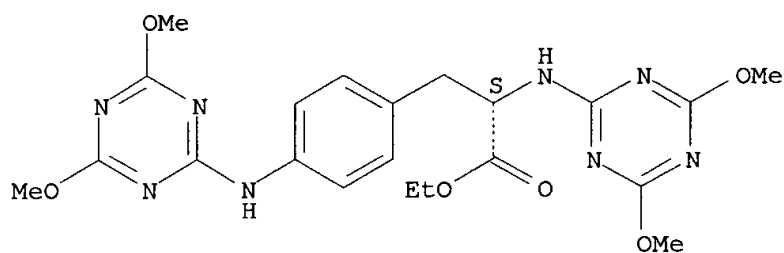
Absolute stereochemistry.



RN 263274-99-3 CAPLUS

CN L-Phenylalanine, N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-[(4,6-dimethoxy-1,3,5-triazin-2-yl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

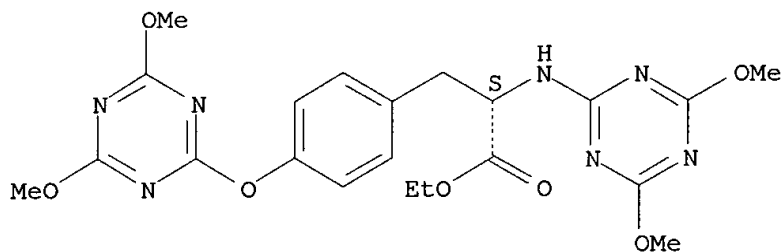
Absolute stereochemistry.



RN 263275-01-0 CAPLUS

CN L-Tyrosine, N,O-bis(4,6-dimethoxy-1,3,5-triazin-2-yl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



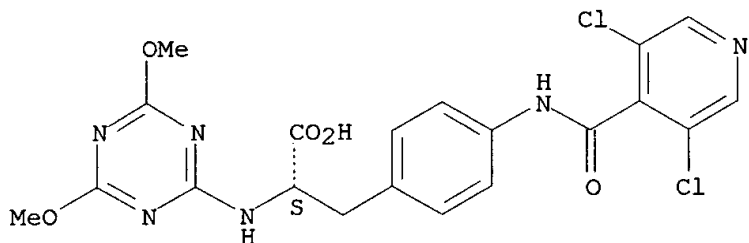
IT 263274-38-0P 263274-67-5P 263274-68-6P
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 263274-90-4P 263274-96-0P 263274-98-2P
 263275-00-9P 263275-02-1P 263275-03-2P
 263275-04-3P

RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of heteroaryl-.beta.-alanine derivs. as antiinflammatory agents and .alpha.4 integrin inhibitors)

RN 263274-38-0 CAPLUS

CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

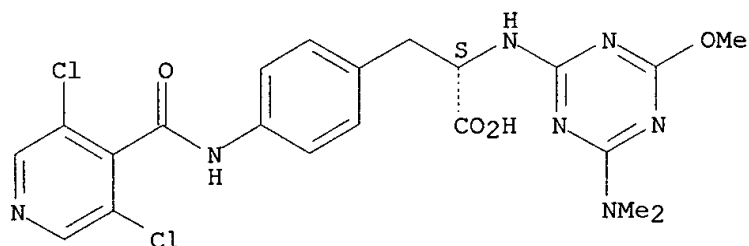
Absolute stereochemistry.



RN 263274-67-5 CAPLUS

CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[4-(dimethylamino)-6-methoxy-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

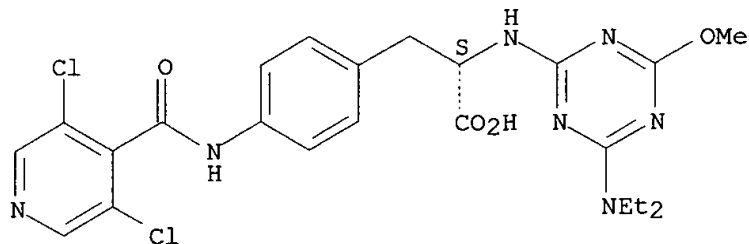
Absolute stereochemistry.



RN 263274-68-6 CAPLUS

CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[4-(diethylamino)-6-methoxy-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

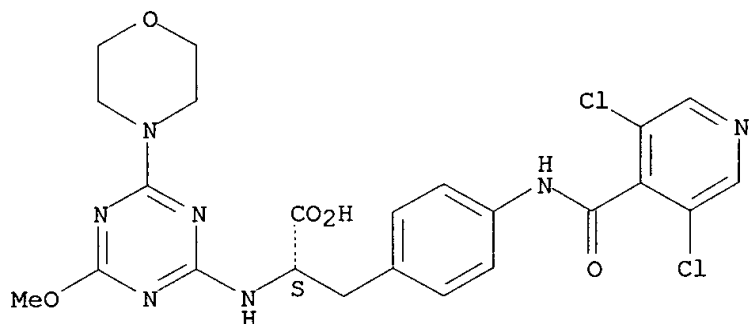
Absolute stereochemistry.



RN 263274-69-7 CAPLUS

CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[4-methoxy-6-(4-morpholinyl)-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

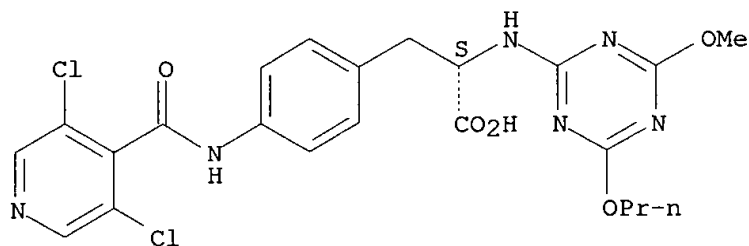
Absolute stereochemistry.



RN 263274-70-0 CAPLUS

CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-(4-methoxy-6-propoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

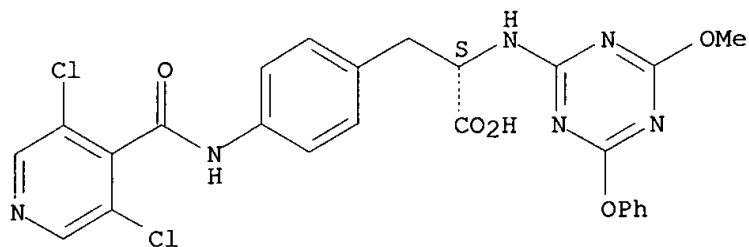
Absolute stereochemistry.



RN 263274-71-1 CAPLUS

CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-(4-methoxy-6-phenoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

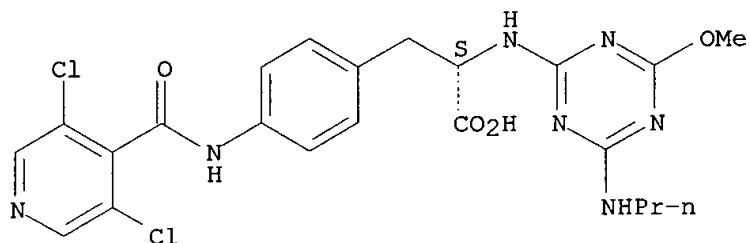
Absolute stereochemistry.



RN 263274-72-2 CAPLUS

CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[4-methoxy-6-(propylamino)-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

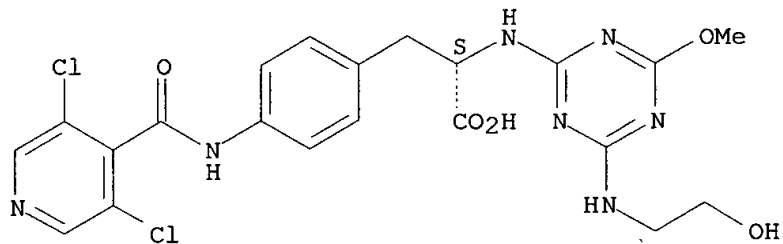
Absolute stereochemistry.



RN 263274-73-3 CAPLUS

CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[4-(2-hydroxyethyl)amino]-6-methoxy-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

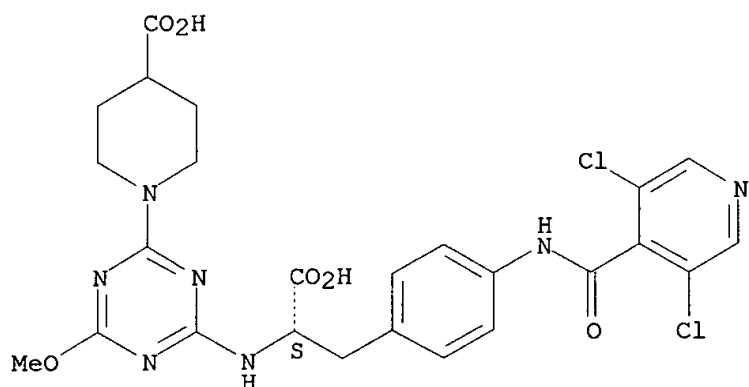
Absolute stereochemistry.



RN 263274-74-4 CAPLUS

CN 4-Piperidinecarboxylic acid, 1-[4-[[(1S)-1-carboxy-2-[4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]phenyl]ethyl]amino]-6-methoxy-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

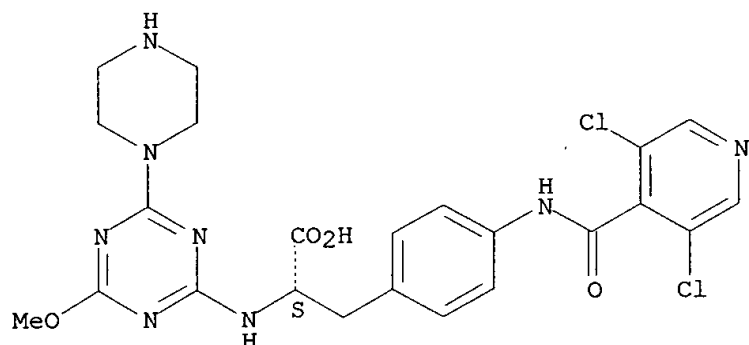
Absolute stereochemistry.



RN 263274-75-5 CAPLUS

CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl) carbonyl] amino]-N-[4-methoxy-6-(1-piperazinyl)-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

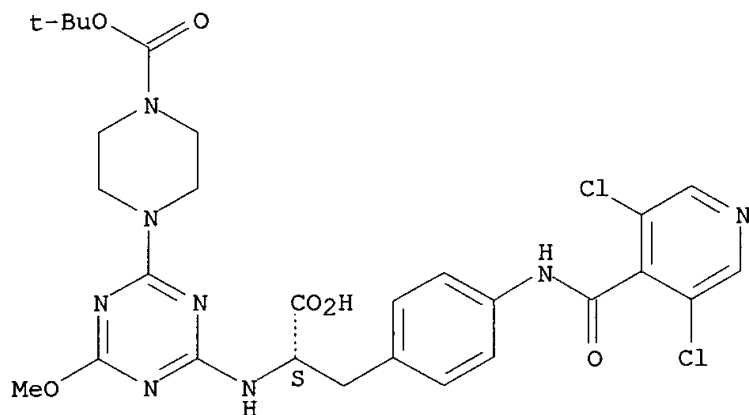
Absolute stereochemistry.



RN 263274-76-6 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[4-[[(1S)-1-carboxy-2-[4-[[(3,5-dichloro-4-pyridinyl) carbonyl] amino] phenyl] ethyl] amino]-6-methoxy-1,3,5-triazin-2-yl]-, 1-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

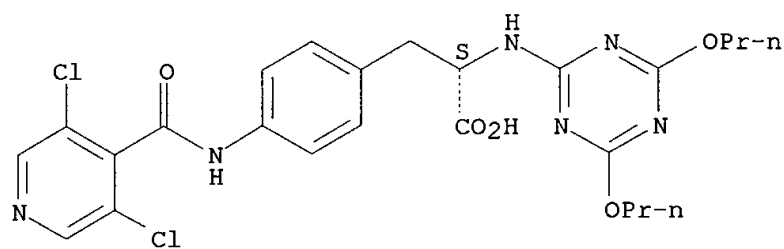
Absolute stereochemistry.



RN 263274-85-7 CAPLUS

CN L-Phenylalanine, 4-[[{(3,5-dichloro-4-pyridinyl)carbonyl}amino]-N-(4,6-dipropoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

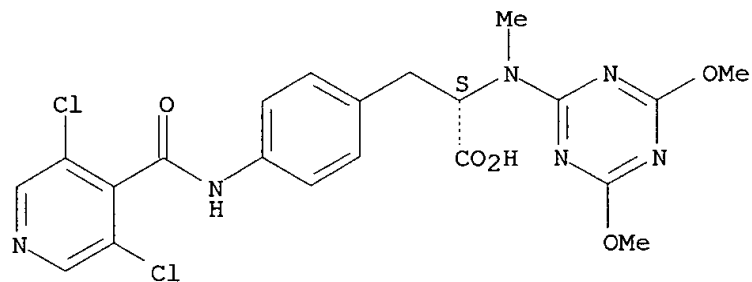
Absolute stereochemistry.



RN 263274-87-9 CAPLUS

CN L-Phenylalanine, 4-[[{(3,5-dichloro-4-pyridinyl)carbonyl}amino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-N-methyl- (9CI) (CA INDEX NAME)

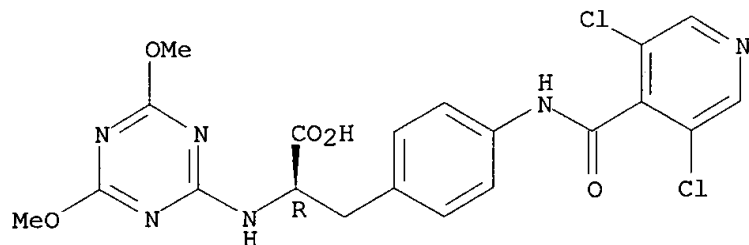
Absolute stereochemistry.



RN 263274-88-0 CAPLUS

CN D-Phenylalanine, 4-[[{(3,5-dichloro-4-pyridinyl)carbonyl}amino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

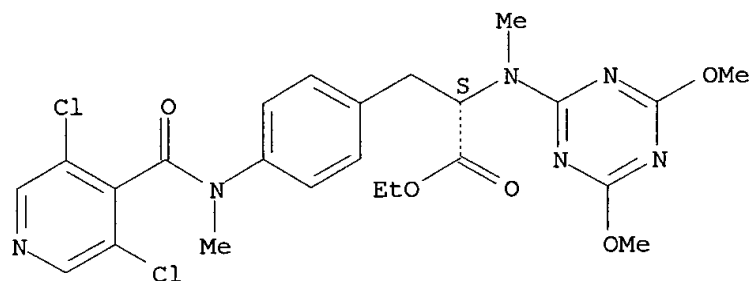
Absolute stereochemistry.



RN 263274-89-1 CAPLUS

CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl) carbonyl] methylamino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-N-methyl-, ethyl ester (9CI) (CA INDEX NAME)

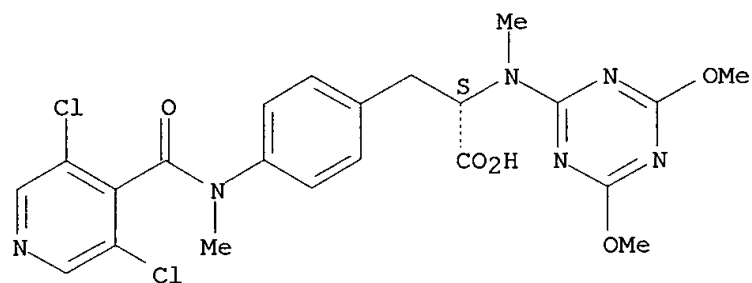
Absolute stereochemistry.



RN 263274-90-4 CAPLUS

CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl) carbonyl] methylamino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-N-methyl- (9CI) (CA INDEX NAME)

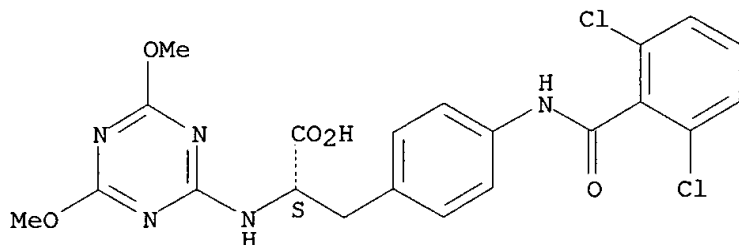
Absolute stereochemistry.



RN 263274-96-0 CAPLUS

CN L-Phenylalanine, 4-[(2,6-dichlorobenzoyl) amino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-N-methyl- (9CI) (CA INDEX NAME)

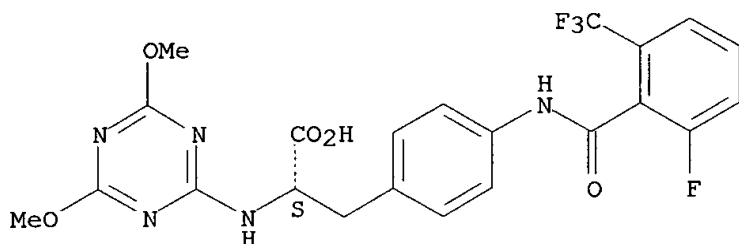
Absolute stereochemistry.



RN 263274-98-2 CAPLUS

CN L-Phenylalanine, N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-[[2-fluoro-6-(trifluoromethyl)benzoyl]amino]- (9CI) (CA INDEX NAME)

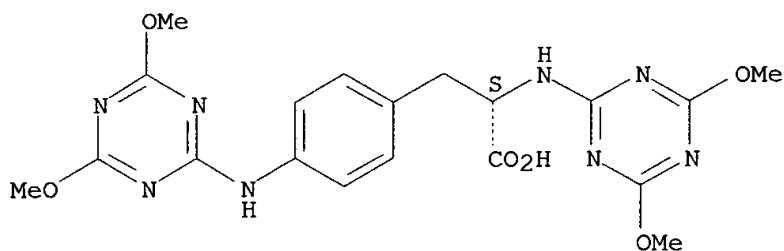
Absolute stereochemistry.



RN 263275-00-9 CAPLUS

CN L-Phenylalanine, N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-[(4,6-dimethoxy-1,3,5-triazin-2-yl)amino]- (9CI) (CA INDEX NAME)

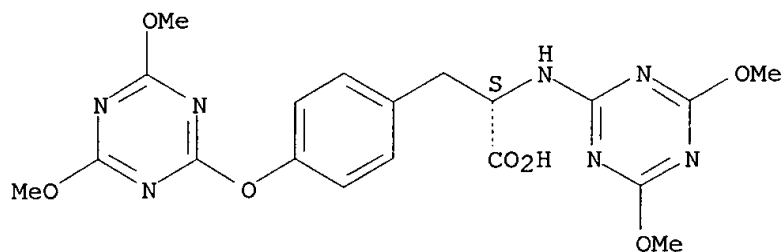
Absolute stereochemistry.



RN 263275-02-1 CAPLUS

CN L-Tyrosine, N,O-bis(4,6-dimethoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

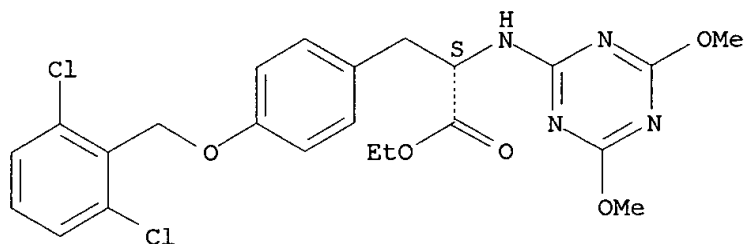
Absolute stereochemistry.



RN 263275-03-2 CAPLUS

CN L-Tyrosine, O-[(2,6-dichlorophenyl)methyl]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-, ethyl ester (9CI) (CA INDEX NAME)

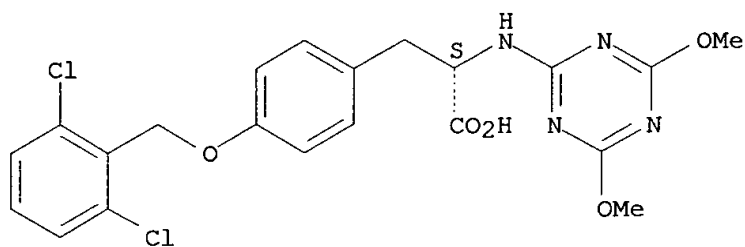
Absolute stereochemistry.



RN 263275-04-3 CAPLUS

CN L-Tyrosine, O-[(2,6-dichlorophenyl)methyl]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



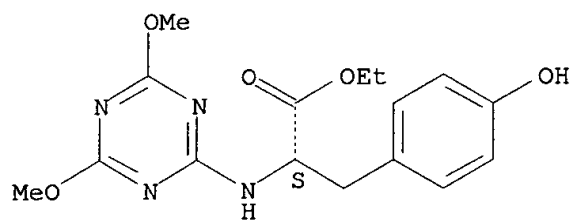
IT 263276-09-1P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of heteroaryl-.beta.-alanine derivs. as antiinflammatory agents and .alpha.4 integrin inhibitors)

RN 263276-09-1 CAPLUS

CN L-Tyrosine, N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L18 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2002 ACS

AN 2002:90026 CAPLUS

DN 136:135019

TI Preparation of 3-amino-2-(4-aminocarbonyloxy)phenyl-propionic acid derivatives as antiinflammatory agents and .alpha.4 Integrin inhibitors

IN Konradi, Andrei W.; Pleiss, Michael A.; Thorsett, Eugene D.; Ashwell, Susan; Welmaker, Gregory S.; Kreft, Anthony; Sarantakis, Dimitrios; Dressen, Darren B.; Grant, Francine S.; Xu, Ying-Zi

PA Elan Pharmaceuticals, Inc., USA; American Home Products Corporation

SO PCT Int. Appl., 137 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

not paid out

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002008206	A1	20020131	WO 2001-US23073	20010720
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2002055509	A1	20020509	US 2001-910685	20010720
PRAI US 2000-220134P	P	20000721		

OS MARPAT 136:135019

AB 3-Amino-2-(4-aminocarbonyloxy)phenyl-propionic acid derivs. I wherein R is a carboxylic acid; R1 and R2 are independently selected from the group consisting of hydrogen, alkyl, substituted alkyl, alkenyl, substituted alkenyl, cycloalkyl, substituted cycloalkyl, or R1 and R2, together with the nitrogen atom to which they are attached, are joined to form an optionally substituted heterocyclic ring provided that said substituted alkyl, substituted alkenyl and substituted cycloalkyl do not carry an aryl, substituted aryl, heteroaryl or substituted heteroaryl group; Ra and R3 are independently a hydrogen or a Me group; R4 and R5 are independently selected from the group consisting of heteroatom group; n is zero or an integer 1; Alk is a straight or branched alkylene chain; Ar is an optionally substituted arom. or heteroarom. group, as well as their pharmaceutical use as .alpha.4.beta.7 Integrin inhibitors for the treatment of inflammatory diseases. Thus, 3-[4-(3,5-dichloropyrid-4-ylcarboxamido)phenyl]-2-(3-chlorophenylamino)propanoic acid was prepd. as .alpha.4 Integrin inhibitor. The preferred compds. of the invention generally have IC50 values in the .alpha.4.beta.1 and .alpha.a.beta.7 assays of 1 .mu.M and below. In the other assays featuring .alpha. integrins of other subgroups the same compds. had IC50 values of 50 .mu.M and above thus demonstrating the potency and selectivity of their action against .alpha.4 integrins. Title compds. were prepd. for treating an inflammatory condition in a mammalian patient which condition is mediated by Very Late Antigen 4 (VLA-4). Inflammatory condition is selected from the group consisting of asthma, Alzheimer's disease, **atherosclerosis**, AIDS dementia, diabetes, inflammatory bowel disease, multiple sclerosis, rheumatoid arthritis, tissue transplantation, tumor metastasis, meningitis, encephalitis, stroke, nephritis, retinitis, atopic dermatitis, psoriasis, myocardial ischemia and acute leukocyte-mediated lung injury.

IT 263274-37-9P 263274-66-4P 263274-86-8P
 263274-93-7P 263274-94-8P 263274-95-9P
 263274-97-1P 263274-99-3P 263275-01-0P

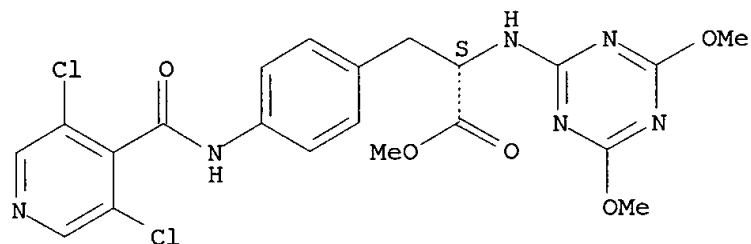
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of aminoaminocarbonyloxyphenylpropionic acid derivs. as a integrin inhibitors)

RN 263274-37-9 CAPLUS

CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-, methyl ester (9CI) (CA INDEX NAME)

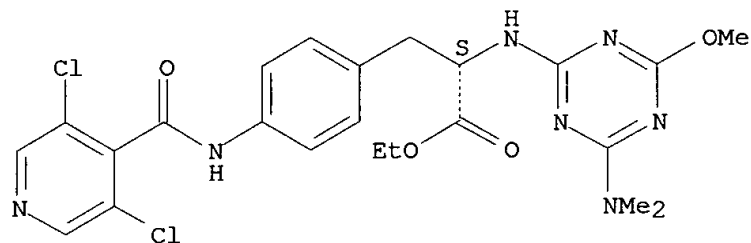
Absolute stereochemistry.



RN 263274-66-4 CAPLUS

CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[4-(dimethylamino)-6-methoxy-1,3,5-triazin-2-yl]-, ethyl ester (9CI) (CA INDEX NAME)

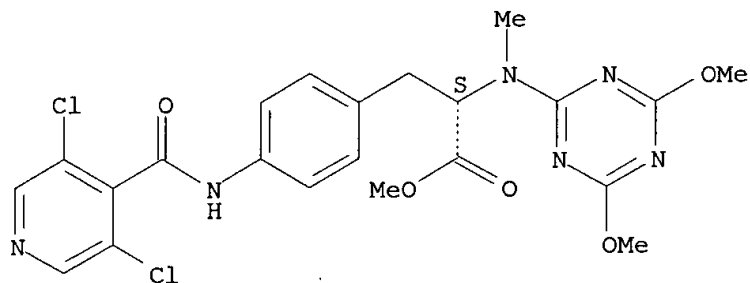
Absolute stereochemistry.



RN 263274-86-8 CAPLUS

CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-N-methyl-, methyl ester (9CI) (CA INDEX NAME)

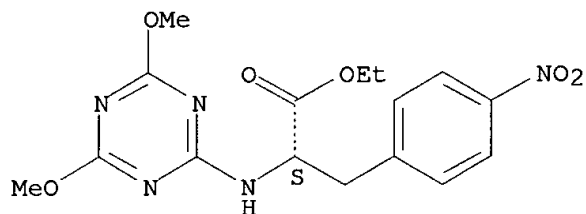
Absolute stereochemistry.



RN 263274-93-7 CAPLUS

CN L-Phenylalanine, N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-nitro-, ethyl ester (9CI) (CA INDEX NAME)

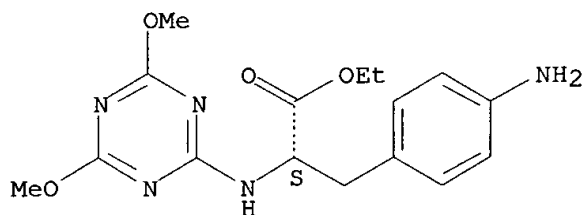
Absolute stereochemistry.



RN 263274-94-8 CAPLUS

CN L-Phenylalanine, 4-amino-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-, ethyl ester (9CI) (CA INDEX NAME)

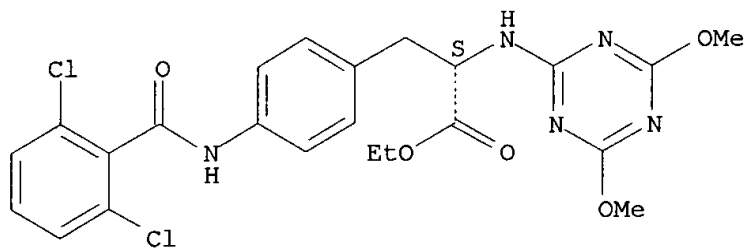
Absolute stereochemistry.



RN 263274-95-9 CAPLUS

CN L-Phenylalanine, 4-[(2,6-dichlorobenzoyl)amino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-, ethyl ester (9CI) (CA INDEX NAME)

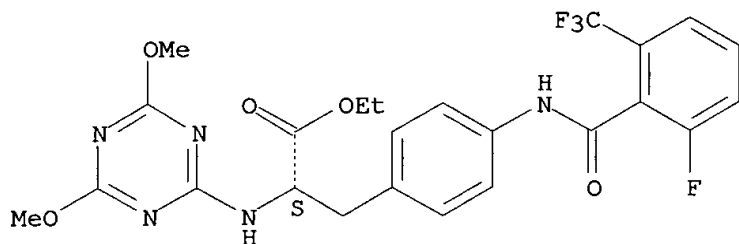
Absolute stereochemistry.



RN 263274-97-1 CAPLUS

CN L-Phenylalanine, N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-[[2-fluoro-6-(trifluoromethyl)benzoyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

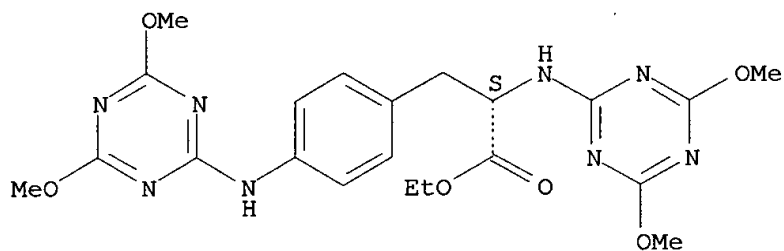
Absolute stereochemistry.



RN 263274-99-3 CAPLUS

CN L-Phenylalanine, N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-[(4,6-dimethoxy-1,3,5-triazin-2-yl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

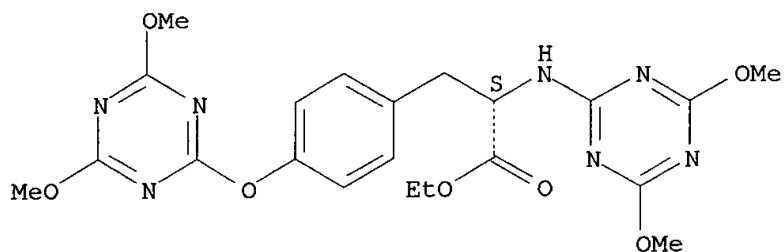
Absolute stereochemistry.



RN 263275-01-0 CAPLUS

CN L-Tyrosine, N,O-bis(4,6-dimethoxy-1,3,5-triazin-2-yl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 263274-38-0P 263274-67-5P 263274-68-6P
 263274-69-7P 263274-70-0P 263274-71-1P
 263274-72-2P 263274-73-3P 263274-74-4P
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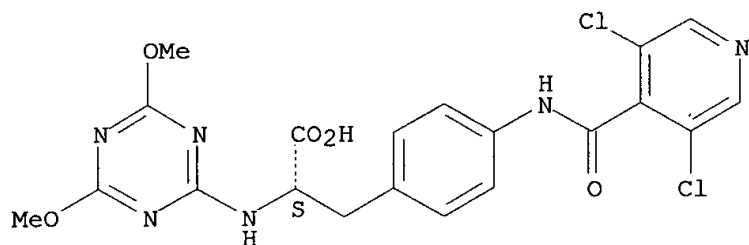
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of aminoaminocarbonyloxyphenylpropionic acid derivs. as a integrin inhibitors)

RN 263274-38-0 CAPLUS

CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

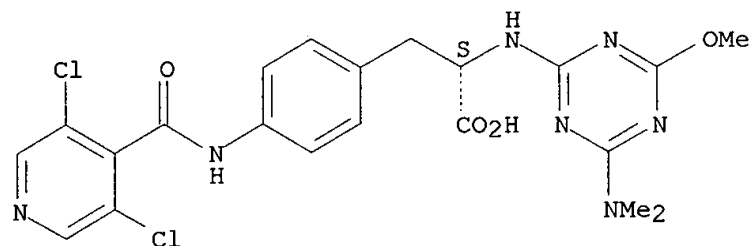
Absolute stereochemistry.



RN 263274-67-5 CAPLUS

CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[4-(dimethylamino)-6-methoxy-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

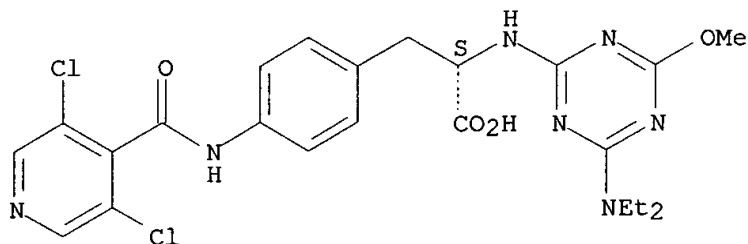
Absolute stereochemistry.



RN 263274-68-6 CAPLUS

CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[4-(diethylamino)-6-methoxy-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

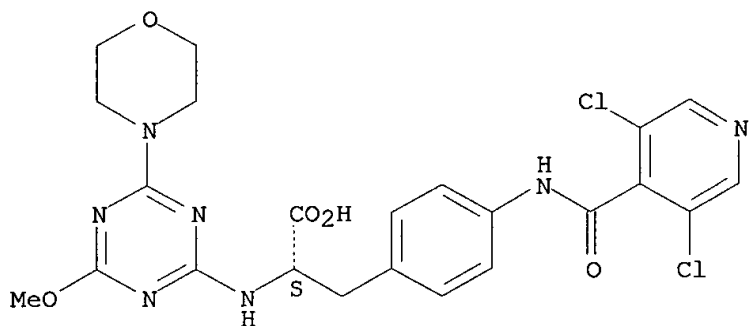
Absolute stereochemistry.



RN 263274-69-7 CAPLUS

CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[4-methoxy-6-(4-morpholinyl)-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

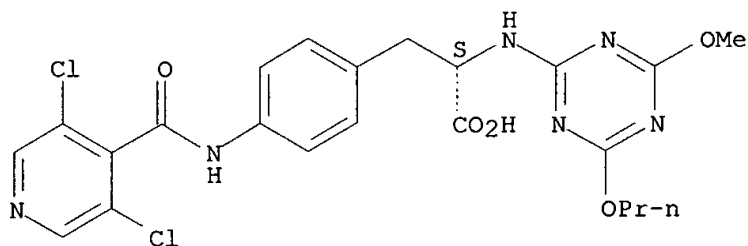
Absolute stereochemistry.



RN 263274-70-0 CAPLUS

CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-(4-methoxy-6-propoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

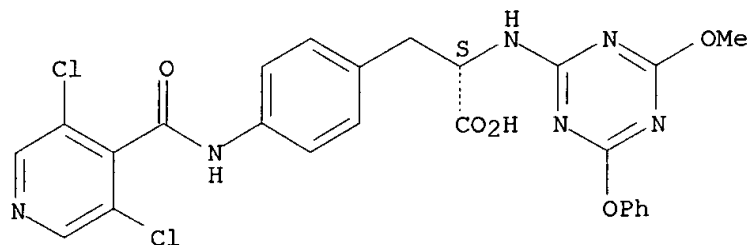
Absolute stereochemistry.



RN 263274-71-1 CAPLUS

CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-(4-methoxy-6-phenoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

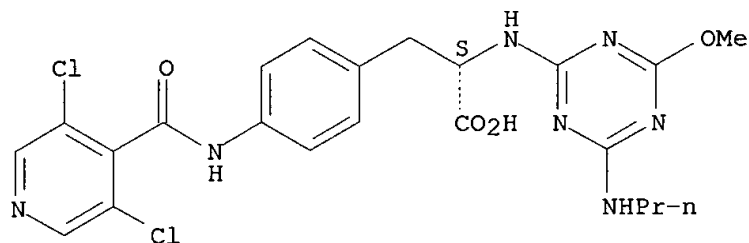
Absolute stereochemistry.



RN 263274-72-2 CAPLUS

CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[4-methoxy-6-(propylamino)-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

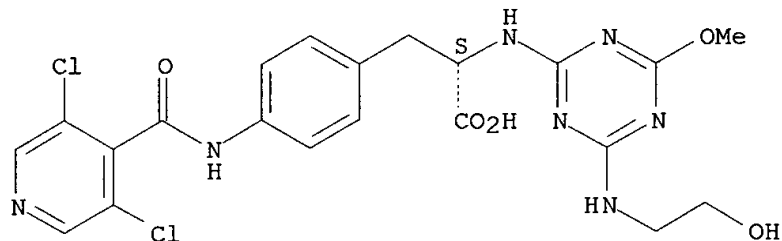
Absolute stereochemistry.



RN 263274-73-3 CAPLUS

CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[4-(2-hydroxyethyl)amino]-6-methoxy-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

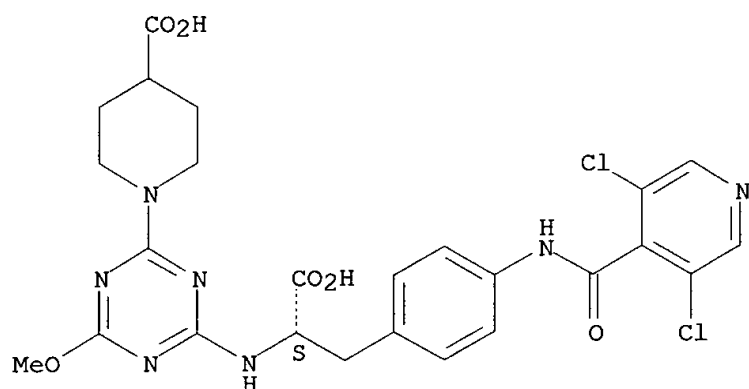
Absolute stereochemistry.



RN 263274-74-4 CAPLUS

CN 4-Piperidinecarboxylic acid, 1-[4-[[(1S)-1-carboxy-2-[4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]phenyl]ethyl]amino]-6-methoxy-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

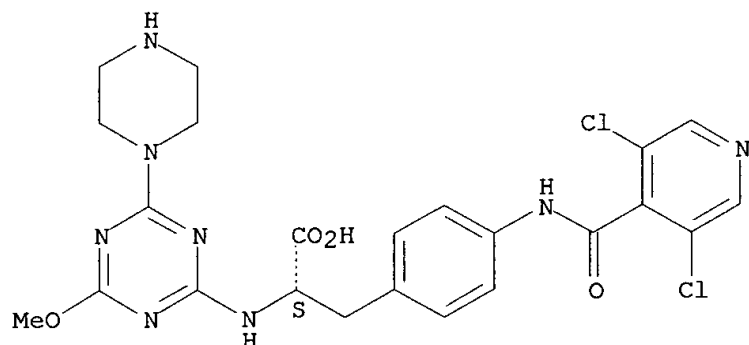
Absolute stereochemistry.



RN 263274-75-5 CAPLUS

CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl) carbonyl] amino]-N-[4-methoxy-6-(1-piperazinyl)-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

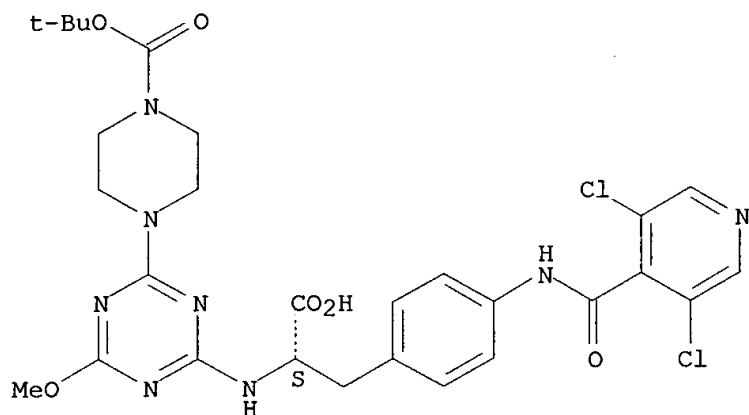
Absolute stereochemistry.



RN 263274-76-6 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[4-[[(1S)-1-carboxy-2-[4-[[(3,5-dichloro-4-pyridinyl) carbonyl] amino] phenyl] ethyl] amino]-6-methoxy-1,3,5-triazin-2-yl]-, 1-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

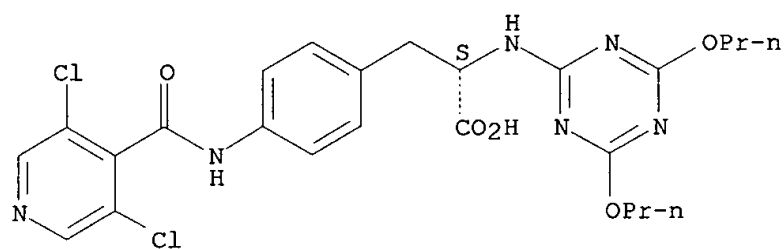
Absolute stereochemistry.



RN 263274-85-7 CAPLUS

CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl) carbonyl] amino]-N-(4,6-dipropoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

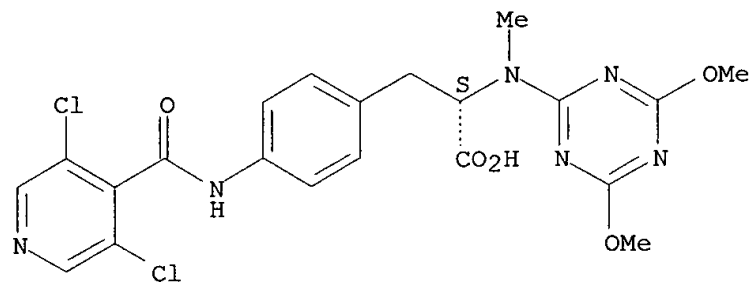
Absolute stereochemistry.



RN 263274-87-9 CAPLUS

CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl) carbonyl] amino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-N-methyl- (9CI) (CA INDEX NAME)

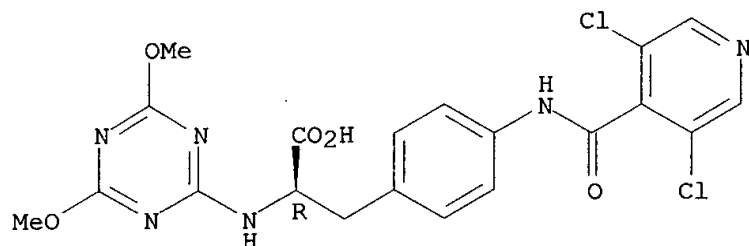
Absolute stereochemistry.



RN 263274-88-0 CAPLUS

CN D-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl) carbonyl] amino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

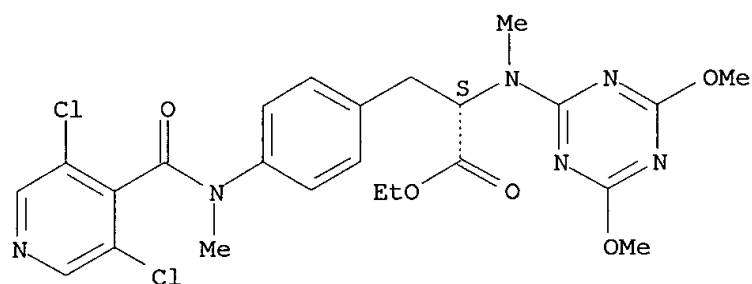
Absolute stereochemistry.



RN 263274-89-1 CAPLUS

CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]methylamino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-N-methyl-, ethyl ester (9CI) (CA INDEX NAME)

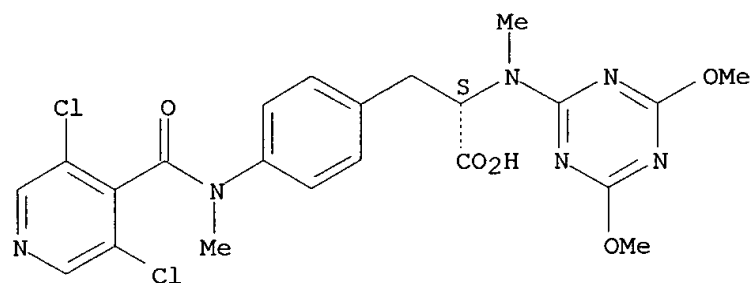
Absolute stereochemistry.



RN 263274-90-4 CAPLUS

CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]methylamino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-N-methyl- (9CI) (CA INDEX NAME)

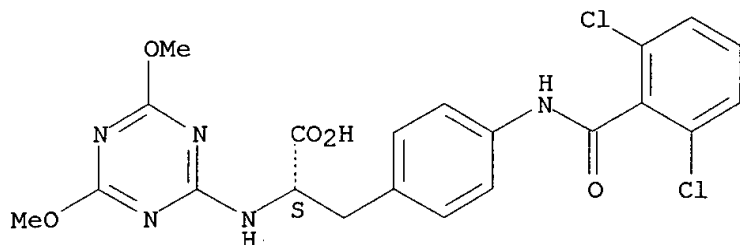
Absolute stereochemistry.



RN 263274-96-0 CAPLUS

CN L-Phenylalanine, 4-[(2,6-dichlorobenzoyl)amino]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-N-methyl- (9CI) (CA INDEX NAME)

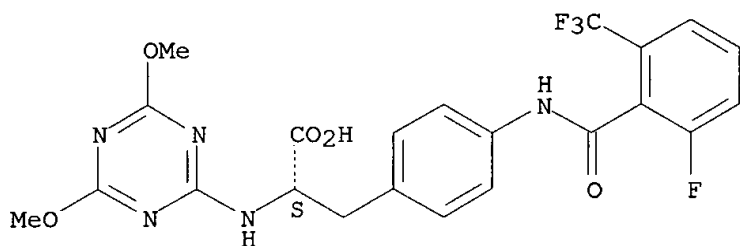
Absolute stereochemistry.



RN 263274-98-2 CAPLUS

CN L-Phenylalanine, N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-[[2-fluoro-6-(trifluoromethyl)benzoyl]amino]- (9CI) (CA INDEX NAME)

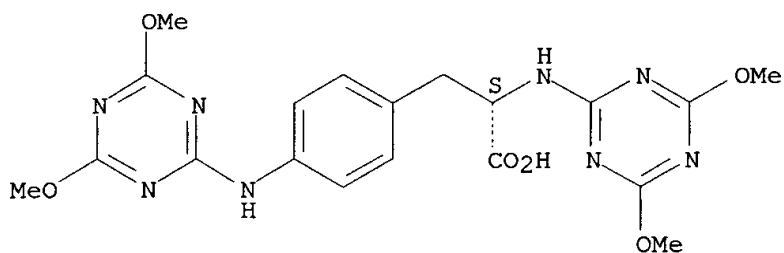
Absolute stereochemistry.



RN 263275-00-9 CAPLUS

CN L-Phenylalanine, N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-[(4,6-dimethoxy-1,3,5-triazin-2-yl)amino]- (9CI) (CA INDEX NAME)

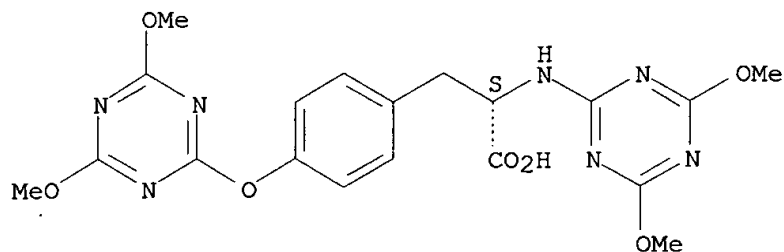
Absolute stereochemistry.



RN 263275-02-1 CAPLUS

CN L-Tyrosine, N,O-bis(4,6-dimethoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

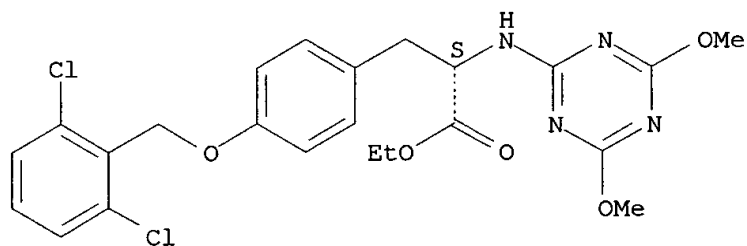
Absolute stereochemistry.



RN 263275-03-2 CAPLUS

CN L-Tyrosine, O-[(2,6-dichlorophenyl)methyl]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-, ethyl ester (9CI) (CA INDEX NAME)

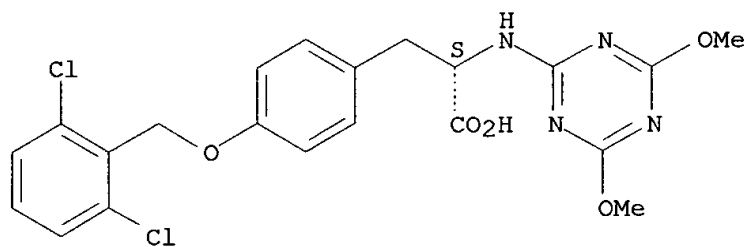
Absolute stereochemistry.



RN 263275-04-3 CAPLUS

CN L-Tyrosine, O-[(2,6-dichlorophenyl)methyl]-N-(4,6-dimethoxy-1,3,5-triazin-2-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



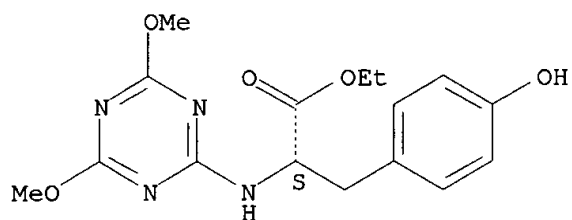
IT 263276-09-1P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of aminoaminocarbonyloxyphenylpropionic acid derivs. as a integrin inhibitors)

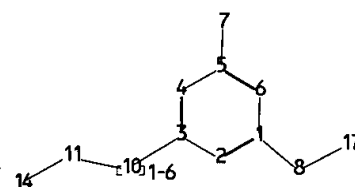
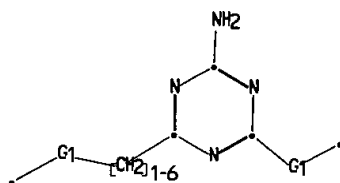
RN 263276-09-1 CAPLUS

CN L-Tyrosine, N-(4,6-dimethoxy-1,3,5-triazin-2-yl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT



chain nodes :

8 10 11

ring nodes :

1 2 3 4 5 6

ring/chain nodes :

7 14 17

chain bonds :

1-8 3-10 5-7 8-17 10-11 11-14

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

1-8 5-7 8-17 10-11 11-14

exact bonds :

3-10

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G1:O,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 10:CLASS 11:CLASS
14:CLASS 17:CLASS

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ENTER SCREEN EXPRESSION OR (END):end

=> screen 2016 OR 2026 OR 2039 OR 2040

L1 SCREEN CREATED

=>

Uploading C:\STNEXP4\QUERIES\10005064 (ex2).str

L2 STRUCTURE UPLOADED

=> que L2 NOT L1

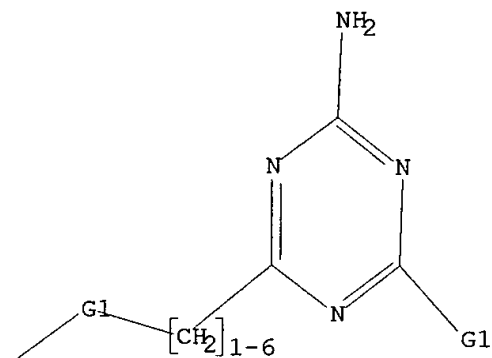
L3 QUE L2 NOT L1

=> d l3

L3 HAS NO ANSWERS

L1 SCR 2016 OR 2026 OR 2039 OR 2040

L2 STR



G1 O,S,N

Structure attributes must be viewed using STN Express query preparation.

L3 QUE L2 NOT L1

=> s l3 sss sam

SAMPLE SEARCH INITIATED 17:40:32 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 862 TO ITERATE

100.0% PROCESSED 862 ITERATIONS

20 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 15479 TO 19001

PROJECTED ANSWERS: 132 TO 668

L4 20 SEA SSS SAM L2 NOT L1

=>Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=> screen 2016 OR 2026 OR 2039 OR 2040

L5 SCREEN CREATED

=>

Uploading C:\STNEXP4\QUERIES\10005064 (ex2).str

L6 STRUCTURE UPLOADED

=> que L6 NOT L5

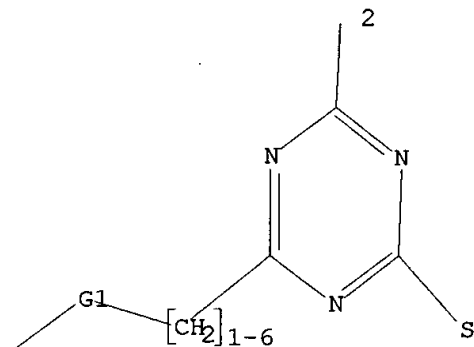
L7 QUE L6 NOT L5

=> d 17

L7 HAS NO ANSWERS

L5 SCR 2016 OR 2026 OR 2039 OR 2040

L6 STR



G1 O,S,N

Structure attributes must be viewed using STN Express query preparation.

L7 QUE L6 NOT L5

=> s 17 sss sam

SAMPLE SEARCH INITIATED 17:42:46 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 28 TO ITERATE

100.0% PROCESSED 28 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 243 TO 877

PROJECTED ANSWERS: 0 TO 0

L8 0 SEA SSS SAM L6 NOT L5

=>Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=> screen 2016 OR 2026 OR 2039 OR 2040

L9 SCREEN CREATED

=>

Uploading C:\STNEXP4\QUERIES\10005064 (ex2).str

L10 STRUCTURE UPLOADED

=> que L10 NOT L9

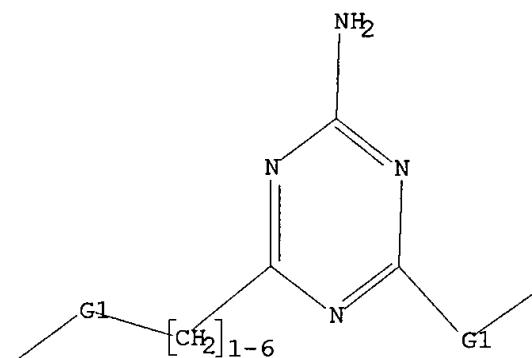
L11 QUE L10 NOT L9

=> d l11

L11 HAS NO ANSWERS

L9 SCR 2016 OR 2026 OR 2039 OR 2040

L10 STR



G1 O,S,N

Structure attributes must be viewed using STN Express query preparation.

L11 QUE L10 NOT L9

=> s l11 sss sam

SAMPLE SEARCH INITIATED 17:44:38 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 696 TO ITERATE

100.0% PROCESSED 696 ITERATIONS

7 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 12338 TO 15502

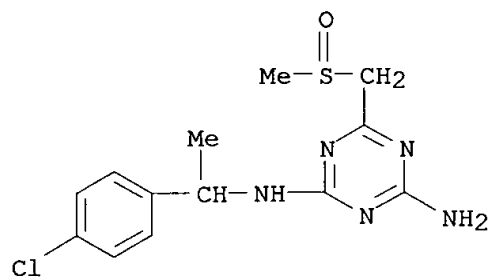
PROJECTED ANSWERS: 7 TO 298

L12 7 SEA SSS SAM L10 NOT L9

10/005,064

=> d scan 112

L12 7 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1,3,5-Triazine-2,4-diamine, N-[1-(4-chlorophenyl)ethyl]-6-
[(methylsulfinyl)methyl]- (9CI)
MF C13 H16 Cl N5 O S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

10/005,064

=> s l11 sss ful
FULL SEARCH INITIATED 17:45:27 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 13319 TO ITERATE

100.0% PROCESSED 13319 ITERATIONS
SEARCH TIME: 00.00.03

187 ANSWERS

L13 187 SEA SSS FUL L10 NOT L9

=> s l13
L14 38 L13

=> d l14 1-38 bib,ab,hitstr

L14 ANSWER 1 OF 38 CAPLUS COPYRIGHT 2002 ACS

AN 2001:680366 CAPLUS

DN 135:366327

TI Synthesis and Biological Evaluation of s-Triazine Substituted Polyamines as Potential New Anti-Trypanosomal Drugs

AU Klenke, Burkhard; Stewart, Mhairi; Barrett, Michael P.; Brun, Reto; Gilbert, Ian H.

CS Welsh School of Pharmacy, Cardiff University, Cardiff, CF10 3XF, UK

SO Journal of Medicinal Chemistry (2001), 44(21), 3440-3452

CODEN: JMCMAR; ISSN: 0022-2623

PB American Chemical Society

DT Journal

LA English

AB The P2 transporter is a nucleoside transporter which is unique to the protozoan parasite *Trypanosoma brucei*, the causative organism of Human African Trypanosomiasis. The transporter has been shown to bind some structural motifs not recognized by other transporters. In this paper we describe the use of the melamine motif, a substrate of the P2 transporter, as a potential tool to selectively deliver polyamine analogs to the parasites. The synthesis of a no. of polyamine analogs attached to a variety of melamine analogs is described. Many of the compds. were shown to competitively inhibit uptake of adenosine, indicating that they are recognized by the transporter. Some of the compds. showed good in vitro activity against the parasites.

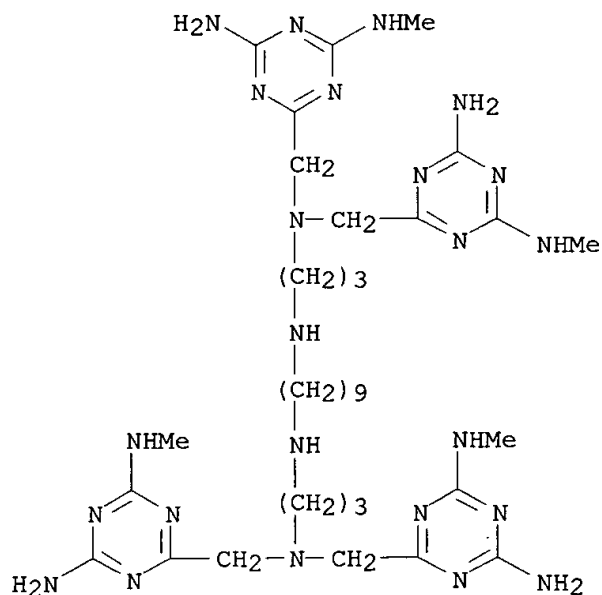
IT 374674-07-4P 374674-10-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. and structure activity relationships of s-triazine substituted polyamines as antitrypanosomal drugs)

RN 374674-07-4 CAPLUS

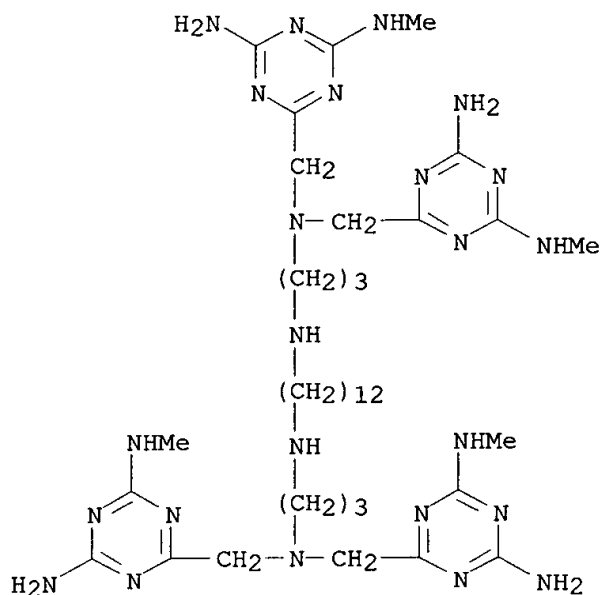
CN 1,3,5-Triazine-2,4-diamine, 6,6',6'',6'''-[1,9-nonanediylbis[imino-3,1-propanediyl]nitrilobis(methylene)]]tetrakis[N-methyl-, heptahydrochloride (9CI) (CA INDEX NAME)



●7 HCl

(Handwritten signature)

RN 374674-10-9 CAPLUS
 CN 1,3,5-Triazine-2,4-diamine, 6,6',6'',6'''-[1,12-dodecanediylbis[imino-3,1-propanediyl]nitrilobis(methylene)]]tetrakis[N-methyl-, heptahydrochloride (9CI) (CA INDEX NAME)



● 7 HCl

RE.CNT 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 2 OF 38 CAPLUS COPYRIGHT 2002 ACS

AN 2001:453092 CAPLUS

DN 135:61555

TI Preparation of lipopeptides as antibacterial agents

IN Hill, Jason; Parr, Ian; Morytko, Michael; Siedlecki, Jim; Yu, Xiang Yang; Silverman, Jared; Keith, Dennis; Finn, John; Christensen, Dale; Lazarova, Tsvetelina; Watson, Alan D.; Zhang, Yan

PA Cubist Pharmaceuticals, Inc., USA; et al.

SO PCT Int. Appl., 202 pp.

CODEN: PIXXD2

DT Patent

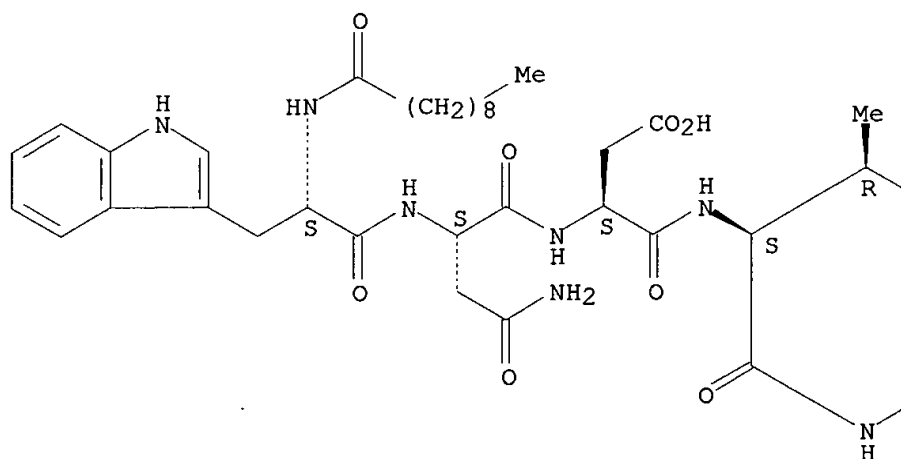
LA English

FAN.CNT 1

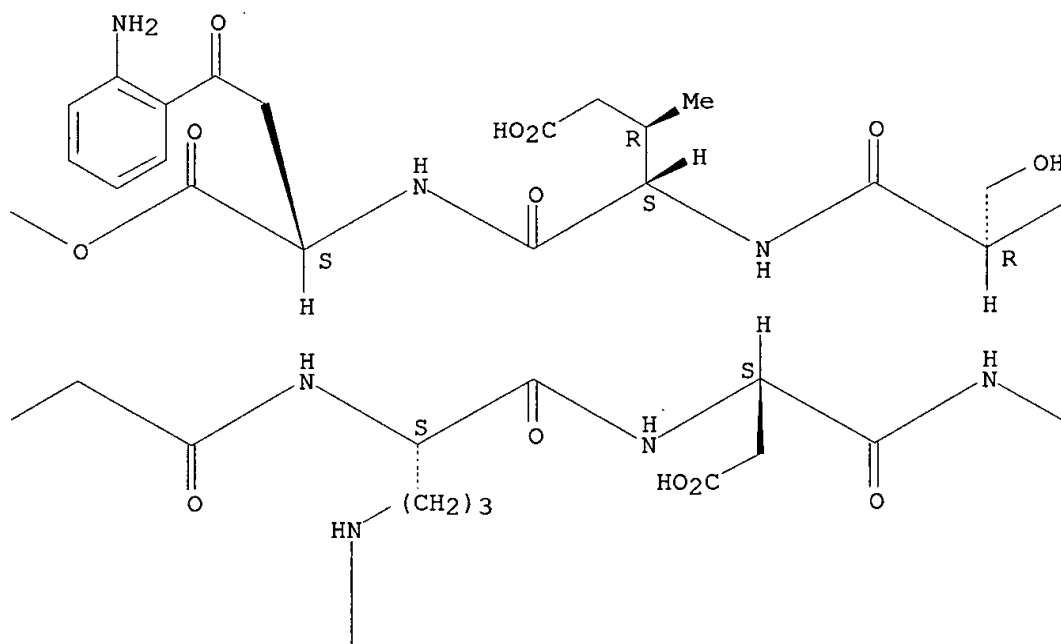
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001044274	A1	20010621	WO 2000-US34205	20001215
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
PRAI	US 1999-170946P	P	19991215		
	US 2000-208222P	P	20000530		
OS	MARPAT 135:61555				
AB	Lipopeptides I [R is -N(B)(X)n-A; B is X''RY, H, alkyl, alkenyl, alkynyl, aryl, heteroaryl, cycloalkyl or heterocyclyl; RY is hydrido, alkyl, alkenyl, alkynyl, aryl, heteroaryl, cycloalkyl, heterocyclyl or hydroxyl; X, X'' are C:O, C:S, C:NH, C:NRX, S:O or SO ₂ ; n is 0 or 1; RX is alkyl, alkenyl, alkynyl, aryl, heteroaryl, cycloalkyl, heterocyclyl, hydroxyl, alkoxy, carboxy or carboalkoxy; A is H, NH ₂ , NHRA, NRARB, heteroaryl, cycloalkyl, heterocyclyl (RA, RB are alkyl, alkenyl, alkynyl, aryl, heteroaryl, cycloalkyl, heterocyclyl or carboalkoxy) or when n is 0, then A is P(O)(OR ₅₀)OR ₅₁ , P(O)R ₅₂ R ₅₃ , or P(O)(OR ₅₀)R ₅₃ , where R ₅₀ -R ₅₃ are alkyl; alternatively B and A may form a 5-7 membered heterocyclic or heteroaryl ring; R ₁ is defined similarly to R (with provisos); R ₂ is CH ₂ CR ₁₇ R ₁₈ -ring, where R ₁₇ and R ₁₈ are hydrido, halo, hydroxyl, alkoxy, amino, thio, sulfinyl, sulfonyl, etc. or CR ₁₇ R ₁₈ are CO, C(:S), oxime or hydrazone group] were prepd. for use as antibacterials. Thus, treating daptomycin with 4-fluorobenzaldehyde and sodium triacetoxyborohydride in dry DMF for 24 h afforded I [R = NHCO(CH ₂) ₈ Me, R ₁ = NHCH ₂ C ₆ H ₄ F-4, R ₂ = CH ₂ COC ₆ H ₄ NH ₂ -o], which showed MIC (S. Aureus) .ltoreq. 1 .mu.g/mL.				
IT	345643-87-0P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of lipopeptides as antibacterial agents)				
RN	345643-87-0 CAPLUS				
CN	Daptomycin, 6-[N5-[[4-amino-6-(phenylamino)-1,3,5-triazin-2-yl]methyl]-L-ornithine]- (9CI) (CA INDEX NAME)				

Absolute stereochemistry.

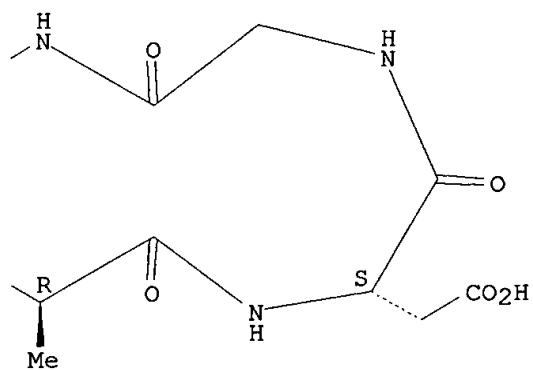
PAGE 1-A



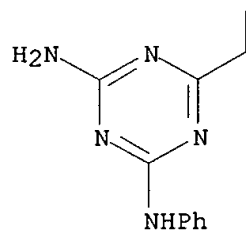
PAGE 1-B



PAGE 1-C



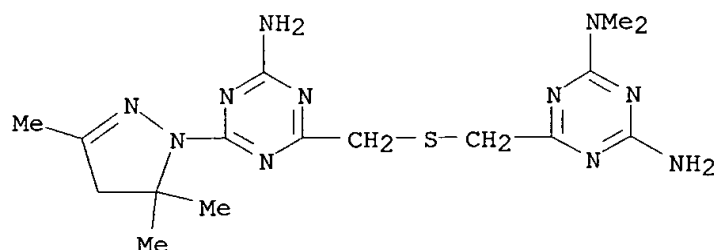
PAGE 2-B



RE.CNT 3

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 3 OF 38 CAPLUS COPYRIGHT 2002 ACS
 AN 2001:87180 CAPLUS
 DN 134:311186
 TI Synthesis, structural characterization and antitumor activity of novel
 2,4-diamino-1,3,5-triazine derivatives
 AU Brzozowski, Z.; Saczewski, F.; Gdaniec, M.
 CS Department of Chemical Technology of Drugs, Medical University of Gdansk,
 Gdansk, P-80-416, Pol.
 SO European Journal of Medicinal Chemistry (2000), 35(12), 1053-1064
 CODEN: EJMCA5; ISSN: 0223-5234
 PB Editions Scientifiques et Medicales Elsevier
 DT Journal
 LA English
 AB The syntheses, structural elucidation and antitumor activities of novel
 2,4-diamino-1,3,5-triazine derivs. are described. The crystal structure
 of one compd., 4-(chloromethyl)-6-(4,5-dihydro-3,5,5-trimethyl-1H-pyrazol-
 1-yl)-1,3,5-triazin-2-amine, was reported. Screenings performed at NCI
 showed that most derivs. possessed a moderate to strong growth inhibition
 activity on various tumor panel cell lines between 0.148 and 56.2 .mu.M
 concns. 4-(Chloromethyl)-6-(4,5-dihydro-3,5,5-trimethyl-1H-pyrazol-1-yl)-
 1,3,5-triazin-2-amine showed the most potent antitumor activity with the
 mean midpoint values of log10 GI50, log10 TGI50 and Log10 LC50 of all
 tests equal to -5.26, -4.81 and -4.37, resp. and therefore, it can be
 considered as a lead structure for further development of anticancer
 agents.
 IT **334993-93-0P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of antitumor diaminotriazines via cyclization of biguanides
 with alkanolic acid esters)
 RN 334993-93-0 CAPLUS
 CN 1,3,5-Triazine-2,4-diamine, 6-[[[4-amino-6-(4,5-dihydro-3,5,5-trimethyl-
 1H-pyrazol-1-yl)-1,3,5-triazin-2-yl]methyl]thio]methyl]-N,N-dimethyl-
 (9CI) (CA INDEX NAME)



RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 5 OF 38 CAPLUS COPYRIGHT 2002 ACS

AN 1999:626180 CAPLUS

DN 131:243289

TI Preparation of 2-[(2-arylthioethyl)amino]-4-amino-1,3,5-triazines as herbicides

IN Kirsten, Rolf; Riebel, Hans-Jochem; Lehr, Stefan; Voigt, Katharina; Kather, Kristian; Dollinger, Markus; Drewes, Mark Wilhelm; Wetcholowsky, Ingo; Watanabe, Yukiyoshi; Goto, Toshio; Myers, Randy Allen

PA Bayer Aktiengesellschaft, Germany; Nihon Bayer Agrochem K.K.

SO PCT Int. Appl., 121 pp.

CODEN: PIXXD2

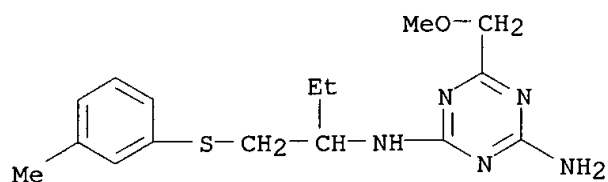
DT Patent

LA German

FAN.CNT 1

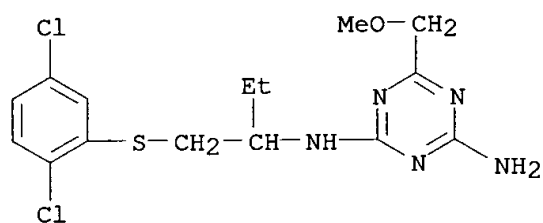
Proviso #2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9948877	A1	19990930	WO 1999-EP1559	19990311
	W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
	DE 19812879	A1	19990930	DE 1998-19812879	19980324
	CA 2325489	AA	19990930	CA 1999-2325489	19990311
	AU 9929328	A1	19991018	AU 1999-29328	19990311
	EP 1064271	A1	20010103	EP 1999-910340	19990311
	R:	AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL			
PRAI	DE 1998-19812879	A	19980324		
	WO 1999-EP1559	W	19990311		
OS	MARPAT 131:243289				
AB	Title compds. [I; n = 0, 1, 2; R1 = H, (substituted) alkyl; R2 = H, formyl, (substituted) alkyl, alkylcarbonyl, alkoxycarbonyl; R3 = (substituted) alkyl, cycloalkyl; R4 = H, alkyl; Ar = (substituted) Ph, naphthyl, heterocyclyl; Z = H, (substituted) alkyl, alkylcarbonyl, alkoxycarbonyl, alkenyl, alkynyl, cycloalkyl], were prepd. Thus, 1-[1-(3-methylphenylthiomethyl)propyl]biguanide hydrochloride and zeolite mol. sieves in MeOH at -10.degree. were treated with NaOMe and Me methoxyacetate followed by 15 h stirring to give 70% 2-amino-4-methoxymethyl-6-[1-(3-methylphenylthiomethyl)propylamino]-1,3,5-triazine. Several I at 250-1000 g/ha preemergent gave complete control of Solanum, Digitaria, Chenopodium, Veronica, etc.				
IT	244264-98-0P 244264-99-1P				
	RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of 2-[(2-arylthioethyl)amino]-4-amino-1,3,5-triazines as herbicides)				
RN	244264-98-0 CAPLUS				
CN	1,3,5-Triazine-2,4-diamine, 6-(methoxymethyl)-N-[1-[(3-methylphenyl)thio]methyl]propyl]- (9CI) (CA INDEX NAME)				



RN 244264-99-1 CAPLUS

CN 1,3,5-Triazine-2,4-diamine, N-[1-[(2,5-dichlorophenyl)thio]methyl]propyl]-6-(methoxymethyl)- (9CI) (CA INDEX NAME)



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

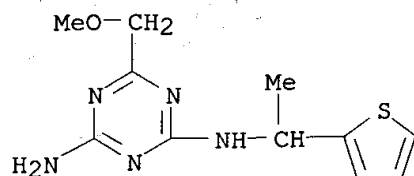
L14 ANSWER 6 OF 38 CAPLUS COPYRIGHT 2002 ACS
 AN 1999:238562 CAPLUS
 DN 130:296699
 TI Preparation of 2,4-diamino-1,3,5-triazines as herbicides
 IN Riebel, Hans-Jochem; Lehr, Stefan; Stelzer, Uwe; Dollinger, Markus;
 Drewes, Mark Wilhelm; Myers, Randy Allen
 PA Bayer A.-G., Germany
 SO Ger. Offen., 36 pp.
 CODEN: GWXXBX
 DT Patent
 LA German
 FAN.CNT 1

Proviso #2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 19744232	A1	19990408	DE 1997-19744232	19971007
	CA 2305806	AA	19990415	CA 1998-2305806	19980924
	WO 9918100	A1	19990415	WO 1998-EP6098	19980924
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	AU 9896280	A1	19990427	AU 1998-96280	19980924
	AU 742963	B2	20020117		
	EP 1021441	A1	20000726	EP 1998-950080	19980924
	R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL				
	BR 9812892	A	20000808	BR 1998-12892	19980924
	JP 2001519348	T2	20011023	JP 2000-514911	19980924
	US 6348435	B1	20020219	US 2000-508383	20000501
PRAI	DE 1997-19744232	A	19971007		
	WO 1998-EP6098	W	19980924		
OS	MARPAT 130:296699				
AB	The title compds. [I; R1 = H, (un)substituted C1-6 alkyl; R2 = H, (un)substituted C1-6 alkyl, COR6; R3 = H, (un)substituted C1-6 alkyl, (un)substituted C2-6 alkenyl or alkynyl, etc; R4 = H, (un)substituted C1-6 alkyl, H, (un)substituted C3-6 cycloalkyl; R5 = H, (un)substituted furyl or thienyl; R6 = (un)substituted C1-6 alkyl(amino), alkoxy, etc.] were prepd., e.g., by reaction of biguanides R1R2NC(:NH)NHC(:NH)NHCR4R5 (R1, R2, R4, R5 as above) or their acid adducts, with alkoxycarbonyl compds. RO2CR3 (R = alkyl, R3 as above). For example, N-deformylation of N-[1-(thien-2-yl)ethyl]formamide (prepn. in 64% yield from 2-acetylthiophene, HCO2H and H2NCHO given) by refluxing with aq. HCl gave 41% 1-(thien-2-yl)ethylamine which was condensed with cyanoguanidine to give 99% 1-[1-(thien-2-yl)ethyl]biguanide.cntdot.HCl. Cyclocondensation of the latter with EtCO2Me in MeOH in the presence of NaOMe gave 32% 2-amino-4-ethyl-6-[1-(thien-2-yl)ethyl]amino-1,3,5-triazine which was N-acetylated with Ac2O to give 45% of a title triazine I (R1 = H, R2 = R4 = Me, R3 = Et, R5 = 2-thienyl) (m. 153.degree.).				
IT	223142-23-2P RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of 2,4-diamino-1,3,5-triazines as herbicides)				
RN	223142-23-2 CAPLUS				
CN	1,3,5-Triazine-2,4-diamine, 6-(methoxymethyl)-N-[1-(2-thienyl)ethyl]-				

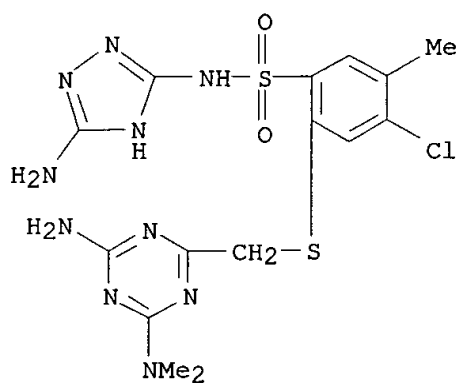
10/005,064

(9CI) (CA INDEX NAME)



6

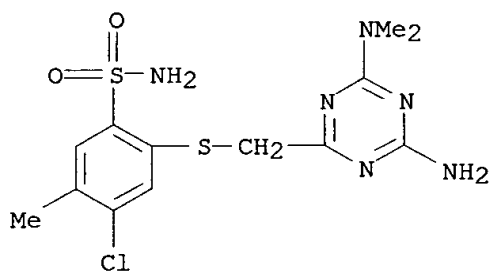
L14 ANSWER 13 OF 38 CAPLUS COPYRIGHT 2002 ACS
 AN 1997:762561 CAPLUS
 DN 128:97298
 TI 2-Mercaptobenzenesulfonamides as novel inhibitors of human
 immunodeficiency virus type 1 integrase and replication
 AU Neamati, N.; Mazumder, A.; Sunder, S.; Owen, J. M.; Schultz, R. J.;
 Pommier, Y.
 CS Lab. Mol. Pharmacol., Div. Basic Sci., Natl. Cancer Inst., Bethesda, MD,
 20892, USA
 SO Antiviral Chem. Chemother. (1997), 8(6), 485-495
 CODEN: ACCHEH; ISSN: 0956-3202
 PB International Medical Press
 DT Journal
 LA English
 AB An obligatory requirement in the retroviral life cycle is the integration
 of the viral dsDNA into the host chromosome, a process performed by viral
 integrase. The retroviral integrase is able to catalyze at least three
 discrete enzymic steps. Two of these steps, 3' processing and DNA strand
 transfer, can be measured in an in vitro assay in the presence of a duplex
 oligonucleotide corresponding to the viral long terminal repeat,
 recombinant integrase and the divalent cations, Mg²⁺ or Mn²⁺. This assay
 provides an efficient means of testing integrase inhibitors. As part of
 our continuous effort in developing novel inhibitors we examd. a series of
 2-mercaptobenzenesulfonamides (MBSAs) for their inhibitory activity
 against human immunodeficiency virus type 1 (HIV-1) integrase. From the
 list of compds. tested in an assay specific for HIV-1 integrase, 26
 compds. inhibited the 3' processing and strand transfer step with 50%
 inhibitory concn. (IC₅₀) values below 25 .mu.M. All the thioether derivs.
 were inactive. These results were further compared with the ability of
 MBSAs to protect HIV-1-infected T4 lymphocyte CEM cells. Among 68 compds.
 tested, 27 exhibited antiviral activity in cell-based assays with
 therapeutic indexes of 1-16. All the MBSAs with antiviral activity were
 also effective inhibitors of recombinant HIV-1 integrase. Several arom.
 disulfides were also tested and found to exhibit moderate antiviral and
 anti-integrase activities. These data demonstrate that MBSAs can be
 developed as inhibitors of HIV-1 integrase with the potential for
 antiviral activity.
 IT **201229-86-9**, NSC 661081 **201229-87-0**, NSC 661082
 RL: BAC (Biological activity or effector, except adverse); BIOL
 (Biological study)
 (structure-activity relations of mercaptobenzenesulfonamides as novel
 inhibitors of HIV-1 integrase and replication)
 RN 201229-86-9 CAPLUS
 CN Benzenesulfonamide, 2-[[[4-amino-6-(dimethylamino)-1,3,5-triazin-2-
 yl]methyl]thio]-N-(5-amino-1H-1,2,4-triazol-3-yl)-4-chloro-5-methyl- (9CI)
 (CA INDEX NAME)



Proviso (new)

RN 201229-87-0 CAPLUS

CN Benzenesulfonamide, 2-[[[4-amino-6-(dimethylamino)-1,3,5-triazin-2-yl]methyl]thio]-4-chloro-5-methyl- (9CI) (CA INDEX NAME)



L14 ANSWER 17 OF 38 CAPLUS COPYRIGHT 2002 ACS
 AN 1990:532221 CAPLUS
 DN 113:132221
 TI Preparation of N-arylsulfonyl-N'-triazinylurea derivatives as herbicides
 IN Levitt, George
 PA du Pont de Nemours, E. I., and Co., USA
 SO U.S., 74 pp. Cont.-in-part of U.S. 4,305,884.
 CODEN: USXXAM
 DT Patent
 LA English
 FAN.CNT 8

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4892946	A	19900109	US 1980-209307	19801124
	US 4394506	A	19830719	US 1979-98781	19791130
	US 4305884	A	19811215	US 1980-171355	19800723
	AU 547325	B2	19851017	AU 1983-13286	19830408
	AU 8313286	A1	19830804		
PRAI	US 1979-98781		19791130		
	US 1980-171355		19800723		
	US 1978-910965		19780530		
	US 1978-965070		19781130		
	US 1979-15341		19790301		
	US 1979-29281		19790413		
	AU 1979-47545		19790529		
	US 1979-49149		19790618		
	US 1980-119165		19800206		

OS MARPAT 113:132221

AB The title urea derivs. [I; R = C1-12 alkoxy, C3-10 alkenyloxy, alkynyloxy, 1-indolinyl, etc.; R2 = NCO, CF3SO2NH, etc.; R3 = H, Me, Cl, Br, F; W = O, S; X = H, Cl, Me, alkoxy, etc.; Y = H, F, Cl, Br, C1-4 alkyl, etc.; Z = N, CH] are prepd. and are useful as herbicides. To a soln. of isocyanate deriv. II in MeCN was added in small portions at room temp. triazine deriv. III to give the urea deriv. I (R = X = MeO, R2 = 5-NCO, R3 = H, W = O, Y = Me, Z = N). Among approx. 50 I prepd. 20 were tested to show pre- and post-emergent herbicidal activity at 0.05 g/ha against a wide variety of weeds.

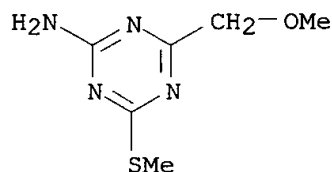
IT 129346-28-7

RL: PROC (Process)

(addn. of, with benzenesulfonyl isocyanate deriv.)

RN 129346-28-7 CAPLUS

CN 1,3,5-Triazin-2-amine, 4-(methoxymethyl)-6-(methylthio)- (9CI) (CA INDEX NAME)



Proviso #4

L14 ANSWER 15 OF 38 CAPLUS COPYRIGHT 2002 ACS
 AN 1996:628531 CAPLUS
 DN 125:275917
 TI Preparation of triazine derivatives as herbicides
 IN Kubota, Mineyuki; Saitou, Masatoshi; Koike, Kazuyoshi; Ogawa, Shin-ichiro
 PA Idemitsu Kosan Co., Ltd., Japan
 SO PCT Int. Appl., 41 pp.
 CODEN: PIXXD2
 DT Patent
 LA Japanese
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9625404	A1	19960822	WO 1996-JP360	19960219
	W: AL, AM, AU, BB, BG, BR, CA, CN, CZ, EE, FI, GE, HU, IS, KG, KR, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	JP 08217763	A2	19960827	JP 1995-29124	19950217
	JP 3029545	B2	20000404		
	CA 2213214	AA	19960822	CA 1996-2213214	19960219
	AU 9646766	A1	19960904	AU 1996-46766	19960219
	AU 699392	B2	19981203		
	EP 810219	A1	19971203	EP 1996-902473	19960219
	EP 810219	B1	20010425		
	R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL				
	CN 1181074	A	19980506	CN 1996-193124	19960219
	AT 200779	E	20010515	AT 1996-902473	19960219
	ES 2158280	T3	20010901	ES 1996-902473	19960219
	US 6004902	A	19991221	US 1997-875786	19971027
PRAI	JP 1995-29124	U	19950217		
	WO 1996-JP360	W	19960219		

OS MARPAT 125:275917

AB The title compds. I [X1 represents linear or branched C1-4 alkyl or halogeno; n represents an integer of 0 to 4, provided that when n is an integer of 2 or above, then X1 substituents may be the same or different; and R1 represents linear or branched C1-10 alkyl optionally having one to four substituents selected from C1-4 alkoxy and/or hydroxy, provided that when the linear or branched C1-10 alkyl is substituted by two or more C1-4 alkoxy groups and/or hydroxy groups, then these substituents may be either the same or different] are prepd. The title triazine derivs. exhibit a very excellent crop/weed selectivity even under severe conditions, for example, excessively humid conditions. The title compd. II at 250 g/ha gave complete control of weeds and caused no damage to wheat.

IT **182194-62-3P**

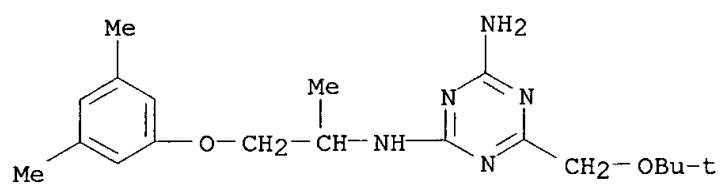
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of triazine derivs. as herbicides)

RN 182194-62-3 CAPLUS

CN 1,3,5-Triazine-2,4-diamine, 6-[(1,1-dimethylethoxy)methyl]-N-[2-(3,5-dimethylphenoxy)-1-methylethyl]- (9CI) (CA INDEX NAME)

Proviso #2
R3 is
only
asked

43 1-1-1



L14 ANSWER 19 OF 38 CAPLUS COPYRIGHT 2002 ACS

AN 1990:138746 CAPLUS

DN 112:138746

TI Preparation of N-arylsulfonyl-N'-arylureas via carbonylation reactions
IN Besenyi, Gabor; Nemeth, Sandor; Simandi, Laszlo; Belak, Maria; Szabo, Maria; Dukai, Jozsef; Nagy, Lajos; Tomordi, Elemer; Soptei, Csaba; Eichhardt Dioszegi, Erzsebet

PA Magyar Tudomanyos Akademia, Kozponti Kemiai Kutato Intezet, Hung.; Nitrokemia Ipartelepek

SO Ger. Offen., 17 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 3906910	A1	19890921	DE 1989-3906910	19890303
	HU 202487	B	19910328	HU 1988-1062	19880304
	AU 8930830	A1	19890907	AU 1989-30830	19890228
	AU 607312	B2	19910228		
	DK 8901002	A	19891002	DK 1989-1002	19890301
	US 4954628	A	19900904	US 1989-317769	19890302
	FR 2628106	A1	19890908	FR 1989-2771	19890303
	FR 2628106	B1	19930604		
	NL 8900534	A	19891002	NL 1989-534	19890303
	GB 2216519	A1	19891011	GB 1989-4946	19890303
	GB 2216519	B2	19911211		
	ES 2010631	A6	19891116	ES 1989-1091	19890303
	JP 02003664	A2	19900109	JP 1989-51808	19890303
	ZA 8901642	A	19900131	ZA 1989-1642	19890303
	DD 279241	A5	19900530	DD 1989-326244	19890303
	PL 152515	B1	19910131	PL 1989-278104	19890303
	CH 678323	A	19910830	CH 1989-797	19890303
	AT 8900482	A	19930715	AT 1989-482	19890303
	AT 397249	B	19940225		
	CN 1038638	A	19900110	CN 1989-102524	19890304
	BR 8901145	A	19891031	BR 1989-1145	19890306
PRAI	HU 1988-1062		19880304		

OS MARPAT 112:138746

AB Ar1SO2NHCONHAr2 [I; Ar1 = (substituted) Ph, naphthyl, thienyl; Ar2 = (substituted) Ph, pyridyl, pyrimidinyl, triazinyl], were prepd. by 1) condensation of Ar1SO2NXY (X = Cl, Br; Y = Na, K, quaternary ammonium, phosphonium) with Ar2NH2 and CO in the presence of a carbonylation catalyst and optionally in the presence of a phase transfer catalyst, 2) condensation of Ar2NXY1 (Y1 = H, Na, K) with Ar1SO2NH2 in the presence of CO, a carbonylation catalyst, and an optional phase transfer catalyst, etc. Thus, 4-MeC6H4SO2NClNa, PdCl2, and MeCN in CH2Cl2 were pressurized to 5.0 MPa CO and the mixt. was stirred 5 h. The product mixt. was stirred 16 h with 2-amino-4-methyl-6-methoxytriazine. Solvent was removed and the residue was stirred with aq. K2CO3 to give 72.5% tosylsulfonyltriazinylurea II.,.

IT 125069-39-8, 2-Amino-4-methoxy-6-methoxymethyltriazine

RL: RCT (Reactant)

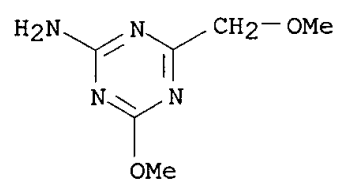
(condensation of, with carbonylated phenylsulfonamide)

RN 125069-39-8 CAPLUS

CN 1,3,5-Triazin-2-amine, 4-methoxy-6-(methoxymethyl)- (9CI) (CA INDEX NAME)

Same as # 16.

10/005,064

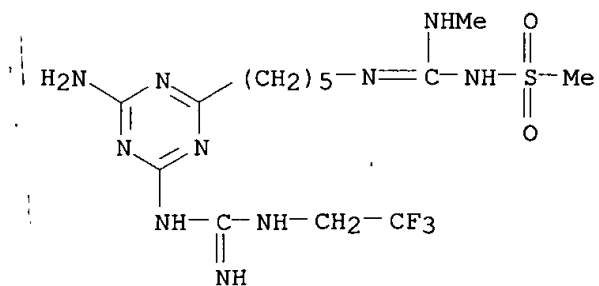


10/005,064

CM 1

CRN 79651-58-4

CMF C14 H25 F3 N10 O2 S



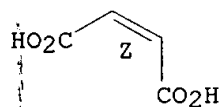
CM 2

CRN 110-16-7

CMF C4 H4 O4

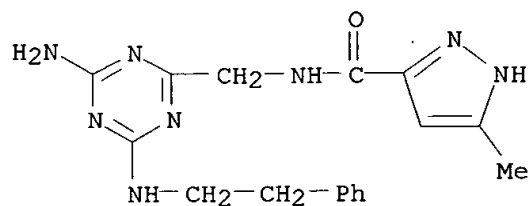
CDES 2:Z

Double bond geometry as shown.

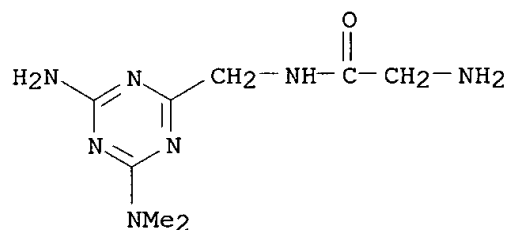


L14 ANSWER 24 OF 38 CAPLUS COPYRIGHT 2002 ACS
 AN 1979:575401 CAPLUS
 DN 91:175401
 TI s-Triazine derivatives
 IN Honna, Ryuji; Ogawa, Kazuo; Toratani, Keiko; Hashimoto, Sadao; Suzue, Takashi
 PA Taiho Yakuhin Kogyo K. K., Japan
 SO Jpn. Kokai Tokkyo Koho, 9 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 FAN.CNT 1

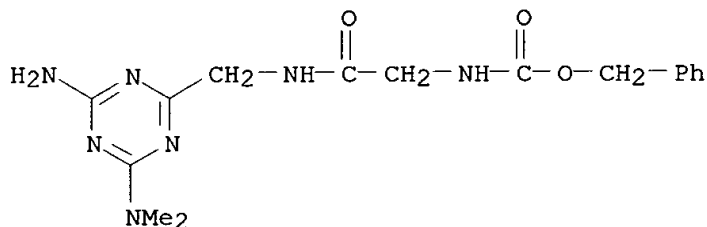
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 54044686	A2	19790409	JP 1977-109107	19770909
	JP 61048516	B4	19861024		
AB	Triazines I [R, R1, Z, Z1 = H, H, O, bond; Me, Me, O, bond; H, Bu, O, bond; H, PhCH2CH2, O, bond; Me, Me, NH, bond; H, Bu, NH, bond; H, H, O, CH2; H, H, O, CH:CH; H, PhCH2CH2, NH, CONHCH2; H, H, O, CONHCH2CH2] and II were prepd., e.g., by reaction of III (R2 = alkoxy) with RR1NC(:NH)NHC(:NH)NH2. Thus, a mixt. of Na, PhCH2CH2NHC(:NH)NHC(:NH)NH2.H Cl, and Me 5-methyl-3-isoxazolecarboxylate in MeOH was refluxed 3 h to give 80.4% II. Hypoglycemic data of II are given in alloxan-diabetic rats.				
IT	71780-11-5P				
	RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)				
RN	71780-11-5 CAPLUS				
CN	1H-Pyrazole-3-carboxamide, N-[[4-amino-6-[(2-phenylethyl)amino]-1,3,5-triazin-2-yl]methyl]-5-methyl- (9CI) (CA INDEX NAME)				



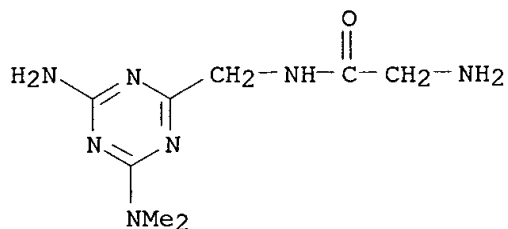
L14 ANSWER 25 OF 38 CAPLUS COPYRIGHT 2002 ACS
 AN 1978:510292 CAPLUS
 DN 89:110292
 TI Mass spectra of triazine derivatives derived from amino acids and peptides
 AU Maekawa, Kazuyuki; Taniguchi, Eiji; Kuwano, Eiichi
 CS Inst. Pflanzenschutz Chem., Univ. Kyushu, Fukuoka, Japan
 SO Org. Mass Spectrom. (1978), 13(1), 4-13
 CODEN: ORMSBG; ISSN: 0030-493X
 DT Journal
 LA German
 AB The mass spectra are reported of 36 triazine derivs. of amino acids and peptides which incorporate the C terminal in the triazine ring. Characteristic fragments indicating the presence of the triazine ring were obsd. which, when used as a marker, enabled estn. of the C-terminal of peptides. In dipeptides both terminals could be detd. simultaneously.
 IT **40917-42-8**
 RL: PRP (Properties)
 (mass spectrum of)
 RN 40917-42-8 CAPLUS
 CN Acetamide, 2-amino-N-[[4-amino-6-(dimethylamino)-1,3,5-triazin-2-yl]methyl]- (9CI) (CA INDEX NAME)



L14 ANSWER 26 OF 38 CAPLUS COPYRIGHT 2002 ACS
 AN 1976:554963 CAPLUS
 DN 85:154963
 TI Pesticides derived from amino acids
 AU Maekawa, K.; Taniguchi, E.; Kuwano, E.; Shuto, Y.
 CS Fac. Agric., Kyushu Univ., Fukuoka, Japan
 SO Environ. Qual. Saf., Suppl. (1975), 3(Pesticides), 748-53
 CODEN: EQSSDX
 DT Journal
 LA English
 AB Benzimidazole derivs. of amino acids and peptides contg. hydrophilic moieties, e.g., benzyloxycarbonylaminomethyl, inhibited the growth of radish seedlings and barnyard grass. 2-(1-Amino-2-phenylethyl)benzimidazole (I) [60603-62-5] (100 ppm) was active against tobacco mosaic virus. 2-[1-(Benzyloxycarbonylamino)-2-(3-indolyl)ethyl]benzimidazole [60603-49-8] and 2-[1-(benzyloxycarbonylamino)-4-guanidylbutyl]benzimidazole [60627-28-3] promoted rice seedling growth but inhibited barnyard grass. Several decarboxylated benzimidazole amino acid derivs. were also fungicidal.
 IT **40917-31-5 40917-42-8 60603-74-9**
 RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)
 (herbicidal and pesticidal activity of)
 RN 40917-31-5 CAPLUS
 CN Carbamic acid, [2-[[[4-amino-6-(dimethylamino)-1,3,5-triazin-2-yl]methyl]amino]-2-oxoethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

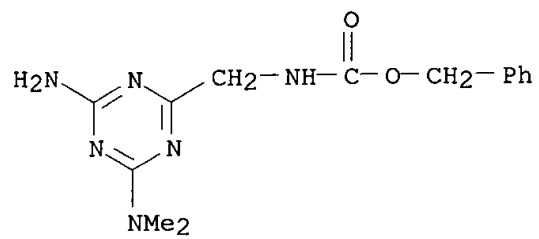


RN 40917-42-8 CAPLUS
 CN Acetamide, 2-amino-N-[[[4-amino-6-(dimethylamino)-1,3,5-triazin-2-yl]methyl]- (9CI) (CA INDEX NAME)



RN 60603-74-9 CAPLUS
 CN Carbamic acid, [[4-amino-6-(dimethylamino)-1,3,5-triazin-2-yl]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

10/005,064



L14 ANSWER 27 OF 38 CAPLUS COPYRIGHT 2002 ACS

AN 1976:180302 CAPLUS

DN 84:180302

TI Cholesterol- and lipid-lowering 2-amino-4-(2-phenylethylamino)-6-(phenoxy)methyl)-1,3,5-triazines

PA Merckle, Ludwig, K.-G., Chem.-Pharm. Fabrik, Fed. Rep. Ger.

SO Brit., 7 pp.

CODEN: BRXXAA

DT Patent

LA English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	GB 1384684	A	19750219	GB 1973-59834	19731227
	DE 2263110	A1	19740711	DE 1972-2263110	19721222
	DE 2263110	B2	19800131		
	DE 2263110	C3	19800918		
PRAI	DE 1972-2263110		19721222		

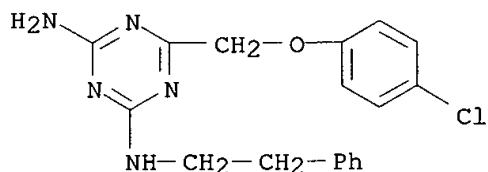
AB Nineteen title compds. I (R = H, Ac, (halophenoxy)alkanoyl; R1, R2 = H, alkyl; R3 = p-halo, o-Cl, m-CF3) were prepd. from Ph(CH2)2NHC(:NH)NHC(:NH)NH2 (II) by treatment with R3C6H4OCR1R2CO2R4 (R4 = H, Et). Thus, I (R = R1 = R2 = H, R3 = p-Cl) was prepd. (82.1%) by treating II in CHCl3 with p-ClC6H4OCH2CO2Et 6 hr at room temp. The cholesterol- and lipid-lowering activities of I were many times greater than that of Clofibrat (no data). LD50 of I were >4 g/kg and >12.5 g/kg for oral administration in rats and mice, resp.

IT 53878-49-2P 53878-55-0P 56367-09-0P
56367-10-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(blood cholesterol and lipids lowering substance, prepn. of)

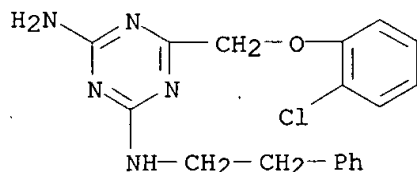
RN 53878-49-2 CAPLUS

CN 1,3,5-Triazine-2,4-diamine, 6-[(4-chlorophenoxy)methyl]-N-(2-phenylethyl)-
(9CI) (CA INDEX NAME)



RN 53878-55-0 CAPLUS

CN 1,3,5-Triazine-2,4-diamine, 6-[(2-chlorophenoxy)methyl]-N-(2-phenylethyl)-
(9CI) (CA INDEX NAME)



RN 56367-09-0 CAPLUS

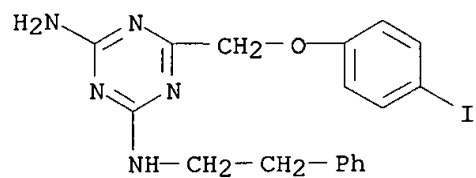
CN 1,3,5-Triazine-2,4-diamine, 6-[(4-iodophenoxy)methyl]-N-(2-phenylethyl)-

*Excluded
from
compd
claims*

Quinon ③

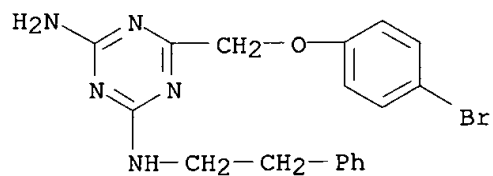
*But
good
for
method*

(9CI) (CA INDEX NAME)

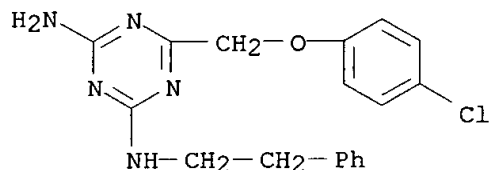


RN 56367-10-3 CAPLUS

CN 1,3,5-Triazine-2,4-diamine, 6-[(4-bromophenoxy)methyl]-N-(2-phenylethyl)-
(9CI) (CA INDEX NAME)

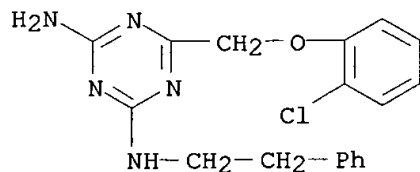


L14 ANSWER 28 OF 38 CAPLUS COPYRIGHT 2002 ACS
 AN 1976:83991 CAPLUS
 DN 84:83991
 TI Hypolipemic activity of clofibrate-related compounds
 AU Metz, G.; Specker, M.
 CS Res. Dev. Dep., L. Merckle K.-G., Blaubeuren, Ger.
 SO Arzneim.-Forsch. (1975), 25(11), 1686-92
 CODEN: ARZNAD
 DT Journal
 LA English
 AB Seventy clofibrate-related compds. with general structures, I, II, III, or IV, were prepd. and their hypolipemic activity was compared to that of clofibrate [637-07-0] in normal and hyperlipemic rats. Many of the compds. were as effective or more effective than clofibrate, and many of them were less toxic than clofibrate. The nature of the acid group seems to be more important for efficacy than the influence of .alpha.-methyl substitution. .alpha.-Substitution seems to be important for the differentiation of anticholesteremic and antitriglyceridemic activity.
 IT **53878-49-2P 53878-55-0P 56367-09-0P 56367-10-3P**
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (prepn. and hypolipemic activity of)
 RN 53878-49-2 CAPLUS
 CN 1,3,5-Triazine-2,4-diamine, 6-[(4-chlorophenoxy)methyl]-N-(2-phenylethyl)-(9CI) (CA INDEX NAME)



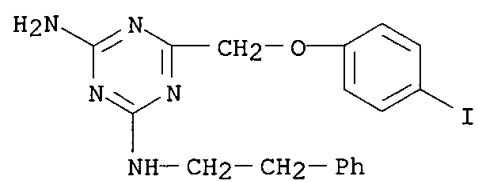
Done on 27

RN 53878-55-0 CAPLUS
 CN 1,3,5-Triazine-2,4-diamine, 6-[(2-chlorophenoxy)methyl]-N-(2-phenylethyl)-(9CI) (CA INDEX NAME)



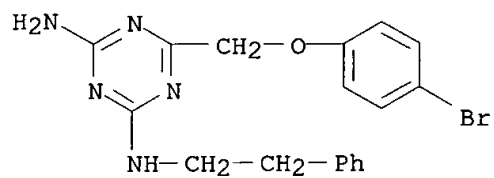
RN 56367-09-0 CAPLUS
 CN 1,3,5-Triazine-2,4-diamine, 6-[(4-iodophenoxy)methyl]-N-(2-phenylethyl)-(9CI) (CA INDEX NAME)

10/005,064

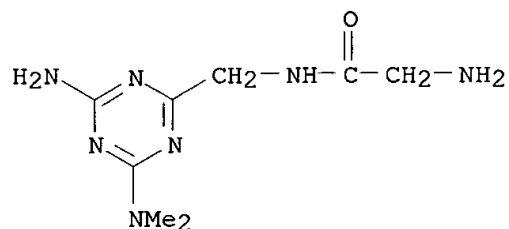


RN 56367-10-3 CAPLUS

CN 1,3,5-Triazine-2,4-diamine, 6-[(4-bromophenoxy)methyl]-N-(2-phenylethyl)-
(9CI) (CA INDEX NAME)



L14 ANSWER 29 OF 38 CAPLUS COPYRIGHT 2002 ACS
 AN 1975:593713 CAPLUS
 DN 83:193713
 TI New method for the determination of peptide carboxyl groups
 AU Maekawa, K.; Kuwano, E.
 CS Inst. Plant Chem., Kyushu Univ., Fukuoka, Japan
 SO Fresenius' Z. Anal. Chem. (1975), 276(2), 121-5
 CODEN: ZACFAU
 DT Journal
 LA German
 AB Treatment of the carboxyl groups of peptides with dimethylbiguanide gave the corresponding peptide-triazines which were hydrolyzed by Streptomyces griseus protease and the amino acid derivs. identified by thin-layer or paper chromatog.
 IT **40917-42-8P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and enzymic hydrolysis of)
 RN 40917-42-8 CAPLUS
 CN Acetamide, 2-amino-N-[[4-amino-6-(dimethylamino)-1,3,5-triazin-2-yl]methyl]- (9CI) (CA INDEX NAME)



L14 ANSWER 31 OF 38 CAPLUS COPYRIGHT 2002 ACS

AN 1974:505580 CAPLUS

DN 81:105580

TI 2-Amino-4-(phenethylamino)-6-(phenoxyalkyl)-1,3,5-triazines

IN Metz, Gunter; Specker, Manfred

PA Merckle, L., K.-G., Chem.-Pharm. Fabrik

SO Ger. Offen., 13 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2263110	A1	19740711	DE 1972-2263110	19721222
	DE 2263110	B2	19800131		
	DE 2263110	C3	19800918		
	AT 7310766	A	19750615	AT 1973-10766	19731221
	AT 328459	B	19760325		
	CH 598235	A	19780428	CH 1973-18096	19731221
	GB 1384684	A	19750219	GB 1973-59834	19731227
PRAI	DE 1972-2263110		19721222		

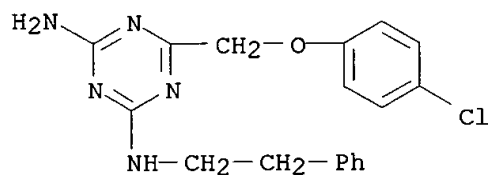
AB Seven triazines (I; Z = CH₂, CH₂CH₂, or CHMeCH₂; R = H, Ac, or COCHMeOC₆H₄Cl-4; R₁ = Cl-2 or -4 or CF₃-3), useful as anticholesteremics and antilipemics (no data), were prepd. by reaction of PhCH₂CH₂NHC(:NH)NHC(:NH)NH₂ (II) with R₁C₆H₄OZCO₂H or their derivs., optionally followed by acylation. LD₅₀ values of I were obtained in the rat. Thus, II reacted with 4-ClC₆H₄OCH₂CO₂Et at room temp. to give 82% I (Z = CH₂, R = H, R₁ = Cl-4), which was also prepd. in 47% yield by refluxing II, 4-ClC₆H₄OCH₂CO₂H, and POCl₃. Re-fluxing I (Z = CH₂CH₂, R = H, R₁ = Cl-4) and Ac₂O gave 60-5% I (Z = CH₂CH₂, R = Ac, R₁ = Cl-4).

IT 53878-49-2P 53878-55-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 53878-49-2 CAPLUS

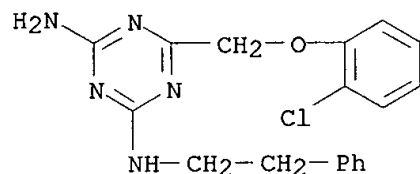
CN 1,3,5-Triazine-2,4-diamine, 6-[(4-chlorophenoxy)methyl]-N-(2-phenylethyl)-
(9CI) (CA INDEX NAME)



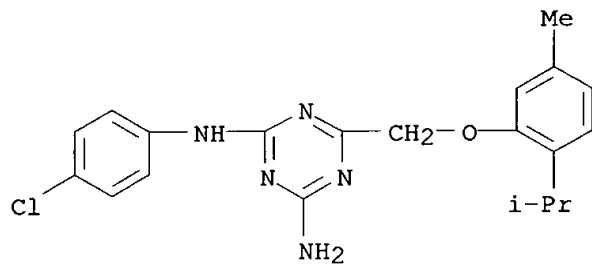
Proviso

RN 53878-55-0 CAPLUS

CN 1,3,5-Triazine-2,4-diamine, 6-[(2-chlorophenoxy)methyl]-N-(2-phenylethyl)-
(9CI) (CA INDEX NAME)

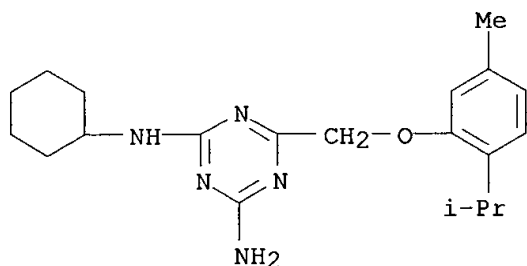


L14 ANSWER 32 OF 38 CAPLUS COPYRIGHT 2002 ACS
 AN 1973:505207 CAPLUS
 DN 79:105207
 TI New substituted triazines and their diuretic activity
 AU Guioa, Mrs. Vas.
 CS Lab. Pharm. Chem., Univ. Athens, Athens, Greece
 SO Ann. Pharm. Fr. (1973), 31(4), 283-92
 CODEN: APFRAD
 DT Journal
 LA French
 AB Triazines I (R = 2,3-(MeO)2C6H3CH2, p-BuC6H4CH:CH, etc.; R1 = H, R2 = Ph, cyclohexyl, Ph(CH2)2, PhCH2, p-ClC6H4; NR1R2 = piperidino, morpholino, 4-methyl-1-piperazino) (48 compds.) were prepd. in 12-77% yields by treating H2NC(:NH)NHC(:NH)NR1R2 (II) with RCO2Et. Thus, II (NR1R2 = morpholino) was heated with 2,3-(MeO)2C6H3CO2Et in presence of MeONa giving 43% I (R = 2,3-(MeO)2C6H3). I (R = 2,3-(MeO)2C6H3, 6,3-(Me2CH)MeC6H4OCH2; NR1R2 = NHC6H4Cl-p) orally had diuretic activity in rats at 10-50 mg/100 g.
 IT **43075-10-1P**
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. and diuretic activity of)
 RN 43075-10-1 CAPLUS
 CN 1,3,5-Triazine-2,4-diamine, N-(4-chlorophenyl)-6-[[5-methyl-2-(1-methylethyl)phenoxy]methyl]- (9CI) (CA INDEX NAME)

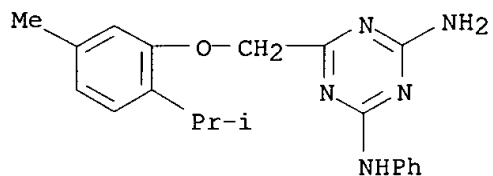


Provin #5

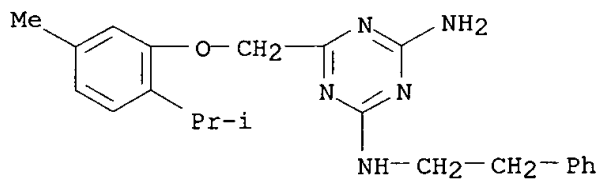
IT **43074-73-3P 43074-78-8P 43075-00-9P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 43074-73-3 CAPLUS
 CN 1,3,5-Triazine-2,4-diamine, N-cyclohexyl-6-[[5-methyl-2-(1-methylethyl)phenoxy]methyl]- (9CI) (CA INDEX NAME)



RN 43074-78-8 CAPLUS

CN 1,3,5-Triazine-2,4-diamine, 6-[[5-methyl-2-(1-methylethyl)phenoxy]methyl]-
N-phenyl- (9CI) (CA INDEX NAME)

RN 43075-00-9 CAPLUS

CN 1,3,5-Triazine-2,4-diamine, 6-[[5-methyl-2-(1-methylethyl)phenoxy]methyl]-
N-(2-phenylethyl)- (9CI) (CA INDEX NAME)

L14 ANSWER 33 OF 38 CAPLUS COPYRIGHT 2002 ACS

AN 1973:160076 CAPLUS

DN 78:160076

TI Synthesis of 1,3,5-triazines from amino acid derivatives. III

AU Kuwano, Eiichi; Taniguchi, Eiji; Maekawa, Kazuyuki

CS Fac. Agric., Kyushu Univ., Fukuoka, Japan

SO Agr. Biol. Chem. (1973), 37(2), 423-30

CODEN: ABCHA6

DT Journal

LA German

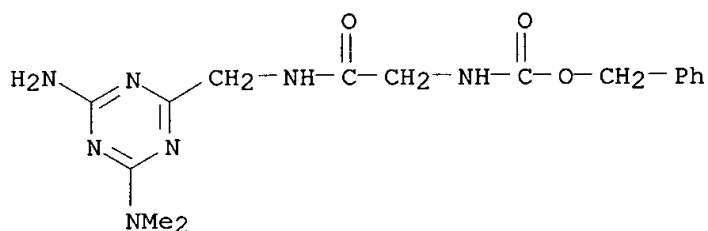
AB Amino acid and peptide esters reacted with $\text{Me}_2\text{NC}(:\text{NH})\text{NHC}(:\text{NH})\text{NH}_2$ (I) to give triazines II. The Me or Et esters could be used as well as reactive esters, such as those of 1-hydroxybenzotriazole or 3-hydroxy-5-methylisoxazole. The reaction proceeded at room temp. Thus, 63% II (R = $\text{PhCH}_2\text{CHNH}_2$) was obtained by treating $\text{PhCH}_2\text{CH}(\text{NH}_2)\text{CO}_2\text{Me}$ with I at room temp. for 2 days. No racemization occurred. When benzyloxycarbonyl-protected dipeptides were used, the protective group could be cleaved with 25% HBr without affecting the triazine ring.

IT 40917-31-5P 40917-42-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

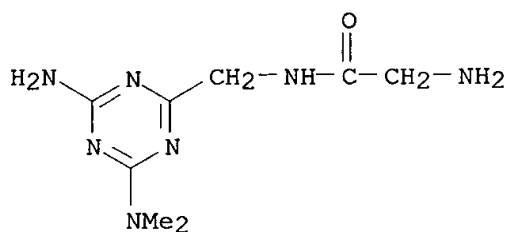
RN 40917-31-5 CAPLUS

CN Carbamic acid, [2-[[[4-amino-6-(dimethylamino)-1,3,5-triazin-2-yl]methyl]amino]-2-oxoethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



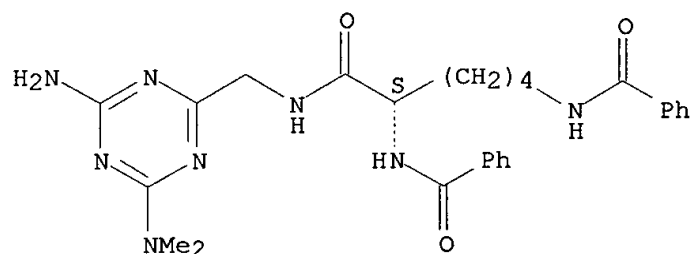
RN 40917-42-8 CAPLUS

CN Acetamide, 2-amino-N-[[4-amino-6-(dimethylamino)-1,3,5-triazin-2-yl]methyl]- (9CI) (CA INDEX NAME)

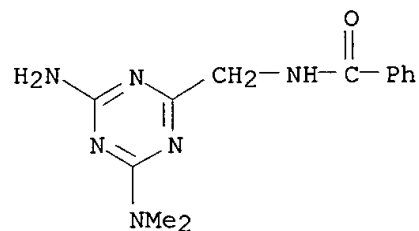


L14 ANSWER 34 OF 38 CAPLUS COPYRIGHT 2002 ACS
 AN 1972:100005 CAPLUS
 DN 76:100005
 TI Synthesis of 1,3,5-triazines from amino acid derivatives. II
 AU Kuwano, Eiichi; Taniguchi, Eiji; Maekawa, Kazuyuki
 CS Fac. Agric., Kyushu Univ., Fukuoka, Japan
 SO Agr. Biol. Chem. (1971), 35(11), 1759-67
 CODEN: ABCHA6
 DT Journal
 LA German
 AB The C-terminal of amino acids and peptides was modified by condensing them with biguanides in the presence of dicyclohexylcarbodiimide. The 1,3,5-triazine derivs. I [R = morpholino, R1 = Me, CH2CH2SMe, CHMe2, CH2Ph, CH2CHMe2, R2 = O2SC6H4Me-p; R = NMe2, R1 = H, Me, CH2Ph, CHMe2, CH2CH2SMe, (CH2)4NHBz, CH2CHMe2, 3-indolylmethyl, R2 = O2SC6H4Me-p, COCH2-NHO2SC6H4Me-p, Bz] were obtained in 54-5% yields.
 IT **35166-15-5**
 RL: PROC (Process)
 (prepn. of)
 RN 35166-15-5 CAPLUS
 CN Benzamide, N,N'-[1-[[[4-amino-6-(dimethylamino)-1,3,5-triazin-2-yl]methyl]amino]carbonyl]-1,5-pentanediy]bis-, (S)- (9CI) (CA INDEX NAME)

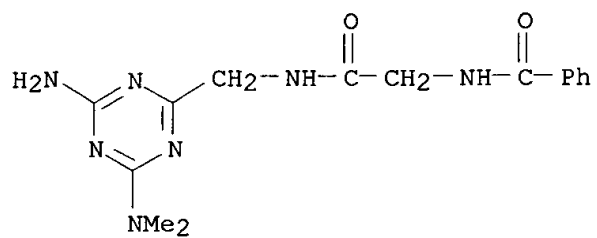
Absolute stereochemistry.



IT **35166-99-5P 35167-09-0P 35167-10-3P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 35166-99-5 CAPLUS
 CN Benzamide, N-[4-amino-6-(dimethylamino)-1,3,5-triazin-2-yl]methyl]- (9CI)
 (CA INDEX NAME)



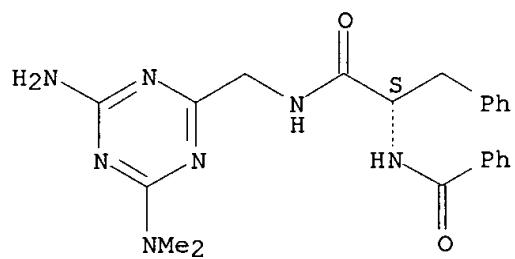
RN 35167-09-0 CAPLUS
 CN Benzamide, N-[2-[[[4-amino-6-(dimethylamino)-1,3,5-triazin-2-yl]methyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)



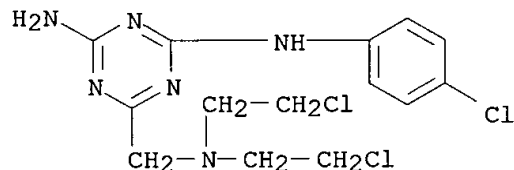
RN 35167-10-3 CAPLUS

CN Benzenepropanamide, N-[[4-amino-6-(dimethylamino)-1,3,5-triazin-2-yl]methyl]-.alpha.-(benzoylamino)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

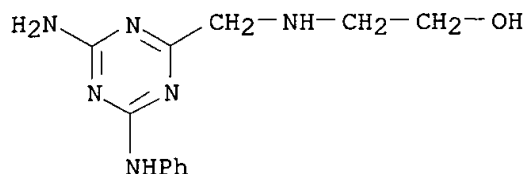


L14 ANSWER 35 OF 38 CAPLUS COPYRIGHT 2002 ACS
 AN 1969:413102 CAPLUS
 DN 71:13102
 TI s-Triazine derivatives
 AU Fel'dman, I. Kh.; Simonov, S. S.
 CS Leningrad. Khim.-Farm. Inst., Leningrad, USSR
 SO Khim. Geterotsikl. Soedin. (1969), (1), 154-6
 CODEN: KGSSAQ
 DT Journal
 LA Russian
 AB I (R = R1 = Cl) (5.4 g.) and 15 g. NH₂C₂H₄OH were heated 1.5 hrs. at 100-10.degree. and cooled and 75 ml. cold H₂O added to yield 5.1 g. I (R = NHC₂H₄OH, R1 = Cl), m. 152-4.degree. (dioxane). Similarly were obtained the following I (X = NHCH₂CH₂OH, Y = N(CH₂CH₂OH)₂, Z = N(CH₂CH₂Cl)₂, Q = NMeNH₂, M = NHNHPh) (R, R1, medium, time (hrs)., temp., m.p., and % yield given): X, H, amine, 1.5, 100-10.degree., 206-8.degree. (dioxane), 71; X, OMe, amine, 1.5, 100-10.degree., 152-4.degree. (dioxane), 64; Y, H, amine, 1.5, 100-10.degree., 121-3.degree. (EtOH), 69.5; Y, Cl, BuOH, 5, reflux, 159-60.degree. (EtOH), 68.0; Y, OMe, BuOH, reflux, 159-61.degree., 66.6; Z, OMe, SOCl₂, 0.5, 40.degree.-50.degree., 180.degree. (EtOH), 54; Z, Cl, SOCl₂, 0.5, 40-50.degree., 183-4.degree. (EtOH), 57.5; Q, H, EtOH, 2.5, reflux, 192-4.degree. (MeOH), 57.2; Q, OMe, EtOH, 2.5, reflux, 199-201.degree. (dioxane), 54; Q, Cl, EtOH, 2.5, reflux, 200-2.degree. (dioxane), 55.4; M, H, EtOH, 2-4, 80-100.degree., 205-7.degree. (dioxane-H₂O), 69.4; M, OMe, iso-PrOH, 2, water bath, 226-7.degree. (dioxane-H₂O), 68.3; M, Cl, EtOH, 2-4, 80-100.degree., 218-19.degree. (BuOH), 72.1.
 IT **22957-62-6P 22957-69-3P 22957-70-6P**
22957-71-7P 22957-72-8P 22957-73-9P
22957-74-0P 22957-75-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 22957-62-6 CAPLUS
 CN s-Triazine, 2-amino-4-[[bis(2-chloroethyl)amino]methyl]-6-(p-chloroanilino)-, monohydrochloride (8CI) (CA INDEX NAME)



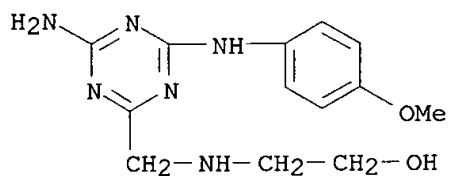
● HCl

RN 22957-69-3 CAPLUS
 CN Ethanol, 2-[[[4-amino-6-anilino-s-triazin-2-yl)methyl]amino]- (8CI) (CA INDEX NAME)



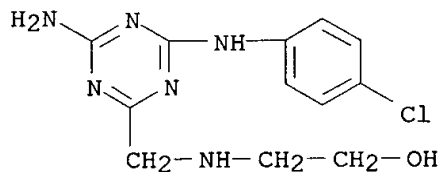
RN 22957-70-6 CAPLUS

CN Ethanol, 2-[[[4-amino-6-p-anisidino-s-triazin-2-yl)methyl]amino]- (8CI)
(CA INDEX NAME)



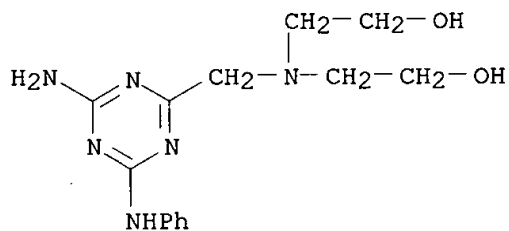
RN 22957-71-7 CAPLUS

CN Ethanol, 2-[[[4-amino-6-(p-chloroanilino)-s-triazin-2-yl)methyl]amino]- (8CI) (CA INDEX NAME)



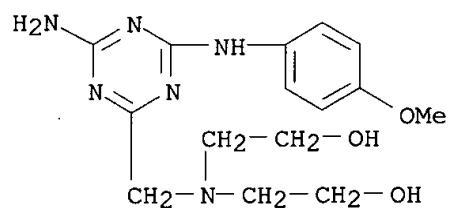
RN 22957-72-8 CAPLUS

CN Ethanol, 2,2'-[[[4-amino-6-anilino-s-triazin-2-yl)methyl]imino]di- (8CI)
(CA INDEX NAME)



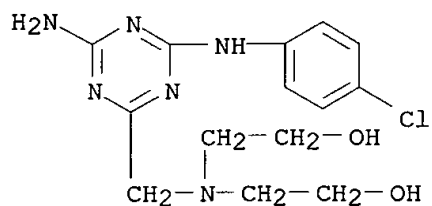
RN 22957-73-9 CAPLUS

CN Ethanol, 2,2'-[[[4-amino-6-p-anisidino-s-triazin-2-yl)methyl]imino]di- (8CI) (CA INDEX NAME)



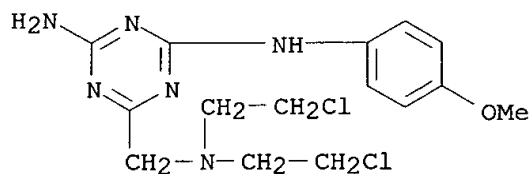
RN 22957-74-0 CAPLUS

CN Ethanol, 2,2'-[[[4-amino-6-(p-chloroanilino)-s-triazin-2-yl]methyl]imino]di- (8CI) (CA INDEX NAME)



RN 22957-75-1 CAPLUS

CN s-Triazine, 2-amino-4-p-anisidino-6-[[bis(2-chloroethyl)amino]methyl]-, monohydrochloride (8CI) (CA INDEX NAME)



● HCl

L14 ANSWER 37 OF 38 CAPLUS COPYRIGHT 2002 ACS

AN 1967:65537 CAPLUS

DN 66:65537

TI Diamino-substituted 1,2-dihydro-1-hydroxy-1,3,5-triazines

PA Upjohn Co.

SO Brit., 22 pp.

CODEN: BRXXAA

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	----	-----	-----	-----
PI	GB 1053113		19661230		
PRAI	US		19630419		

AB The title compds. (I) were prepd. by the reaction of a biguanide with a deriv. of a carboxylic acid to give a triazine (II) which is then oxidized with a perbenzoic acid to give I. Thus, a soln. of 4.6 g. Na in 100 ml. MeOH was added to 21.8 g. 1,1-diallylbiguanide-HCl in 50 ml. MeOH at 25.degree., 74. g. EtO₂CH added, and the mixt. stirred 48 hrs. to give 11.6 g. II (R = H), m. 113-16.degree.. II (R = H) (5.1 g.) in 150 ml. EtOH was treated over 20 min. with 6.9 g. BzOOH in 50 ml. EtOH and the mixt. stirred 18 hrs. at 0.5.degree. to give 2.3 g. I (R = H), m. 139-41.degree.. Similarly prepd. were: II (R = Me), m. 81-2.degree.; I (R = Me), m. 132-4.degree.. Hydrogenation of I (R = Me) over PtO₂ in EtOH gave the corresponding dipropylamino analog, m. 145-7.degree.. I and II similarly prepd., but using m-ClC₆H₄CO₂OH in the oxidn., were (R, II m.p., and I m.p. given): Et, 65-6.degree., 108.5-10.degree.; PhCH₂, 58-60.degree.; oil; Bu, 32-4.degree., 82-5.degree.; cyclohexyl, 90-2.degree., 139-42.degree.; Ph, 82-4.degree., 135-45.degree.; MeOCH₂CH₂, - (b0.2-0.7 144-60.degree.), 132-4.degree.; Me(MeO)CHCH₂, - (b0.25-0.40 145-7.degree.), - (non-cryst. oil); vinyl, 64-5.degree., - (non-cryst. oil); Pr, 50-2.degree., 88-91.degree.; iso-Pr, 49-51.degree., 119-21.degree.; n-pentyl, - (b1 155-7.degree.), - (non-cryst. oil); p-ClC₆H₄, 87-9.degree., 65-80.degree. (non-cryst.); PhCH₂CH₂, - (b0.3 180-2.degree.), 118-20.degree.; Ph(CH₂)₃, 57-60.degree., 91-3.degree.; cyclopropyl, 55-7.5.degree., 104-6.degree.. Similarly prepd. from 1,1-(3-oxapentamethylene)biguanide-HCl were 2-amino-4-methyl-6-morpholino-1,3,5-triazine, m. 184-5.degree., and 1,2-dihydro-1-hydroxy-2-imino-6-methyl-4-morpholino-1,3,5-triazine, m. 254-5.degree.. 2,4-Dichloro-6-methyl-1,3,5-triazine (16.4 g.) in Et₂O was added over 90 min. at 0-5.degree. to 11.4 g. allylamine in Et₂O to give 11.9 g. 2-allylamino-4-chloro-6-methyl-1,3,5-triazine, m. 53-6.degree.. This product was heated 2 hrs. at 100.degree. with diallylamine in Me₂NCHO to give 2-allylamino-4-diallylamino-6-methyl-1,3,5-triazine, m. 40-1.5.degree., which was oxidized with m-ClC₆H₄-CO₂OH to give 1,2-dihydro-1-hydroxy-2-allylimino-4-diallylamino-6-methyl-1,3,5-triazine, m. 78-80.degree.. Similarly prepd. were: 2-anilino-4-chloro-6-methyl-1,3,5-triazine, m. 100-15.degree.; 2-anilino-4-diallylamino-6-methyl-1,3,5-triazine, b1.1 180-95.degree.; 1,2-dihydro-1-hydroxy-4-diallylamino-6-methyl-2-phenylimino-1,3,5-triazine, m. 103-5.degree.; 2-benzylamino-4-chloro-6-methyl-1,3,5-triazine, m. 98-100.degree.; 2-benzylamino-4-diallylamino-6-methyl-1,3,5-triazine, m. 67-9.degree.; 1,2-dihydro-1-hydroxy-2-benzylimino-4-diallylamino-6-methyl-1,3,5-triazine, m. 84-6.degree.. Ir and uv spectra were given for most of the compds. prepd. The title compds. and their salts are active orally and parenterally as antihypertensives with vasodilatory activity, antisecretory agents, and central nervous system depressants. The title compds. are also intermediates in the prepn. of resins, and their salts

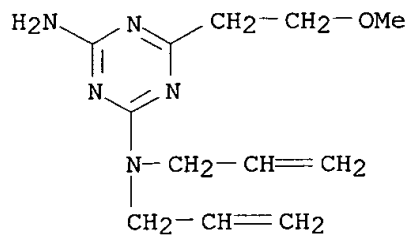
with fluorosilicic acid are mothproofing agents.

IT **5122-68-9P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 5122-68-9 CAPLUS

CN s-Triazine, 2-amino-4-(diallylamino)-6-(2-methoxyethyl)- (7CI, 8CI) (CA
INDEX NAME)



L14 ANSWER 38 OF 38 CAPLUS COPYRIGHT 2002 ACS
 AN 1967:65524 CAPLUS
 DN 66:65524
 TI 1,2-Dihydro-1-hydroxy-1,3,5-triazines
 IN Ursprung, Joseph J.
 PA Upjohn Co.
 SO U.S., 17 pp.
 CODEN: USXXAM
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3270015		19660830	US	19630419
AB	<p>The title compds. of structure I are prepd. and are orally and parenterally active in birds and mammals, have vasodilatory activity, and are useful for lowering the blood pressure and for treatment of shock. I may be used as free base or as salts of pharmacol. accepted acids. I are prepd. by oxidn. of the proper triazine (II) with a 0-5-substituted peroxybenzoic acid (III). II are prepd. from appropriated biguanides which in turn are prepd. by treating a cyanoguanidine, NCNHC(:NH)NHR₃ with a suitable R₂H.HCl or by treating R₂C(:NH)NHCN with R₃NH₂.HCl. II can also be prepd. by treating cyanuric chloride with 1 mole R₁MgX to give the dichloro-s-triazine (IV) which is then treated with 1 equiv. NH₃ or primary amine and with 1 equiv. secondary amine or vice versa. II may be also prepd. by treating V first with NH₃ or a primary amine and then with a secondary amine. The oxidn. of II with III is carried out by mixing the reagents in an inert solvent at below 50.degree., preferably at -10 to 10.degree.. I may be isolated from the reaction mixt. by filtration, extn., or chromatography. MeONa from 4.6 g. Na in 100 ml. MeOH was added with stirring to 21.8 g. 1,1-diallylbiquanide-HCl (VI) in 50 ml. MeOH at 25.degree., 7.4 g. HCO₂Et added, the mixt. stirred 48 hrs. at 25.degree. and evapd. in vacuo, and H₂O added to cause the sepn. of 11.6 g. 2-amino-4-diallylamino-1,3,5-triazine (VII), m. 113-16.degree. (EtOH-H₂O). BzOOH (6.9 g.) in 50 ml. EtOH was added gradually (20 min.) to 5.1 g. VII in 150 ml. EtOH at 5.degree., the mixt. stirred 18 hrs. at 0-5.degree. and evapd. in vacuo, the ppt. filtered off and washed with H₂O, and the combined filtrates extd. with CHCl₃ to give 1,2-dihydro-1-hydroxy-4-diallylamino-2-imino-1,3,5-triazine (VIII), m. 139-41.degree.. Addn. of 1 equiv. HCl in abs. EtOH gave the VIII.HCl salt; addn. of 2 equivs. HCl gave the VIII.2HCl salt. With EtOAc in lieu of HCO₂Et the 6-Me deriv. (IX) of VII, m. 81-2.degree., was obtained. IX oxidized with BzOOH gave the 6-Me deriv. (X) of VIII, m. 132-4.degree.. Hydrogenation of X in EtOH over PtO₂ at 50 lb. H and 25.degree. gave the 4-dipropylamino analog of X, m. 145-7.degree. (MeCN). VI (87 g.) in 300 ml. MeOH, MeONa (from 18.4 g. Na and 300 ml. MeOH), and 44.9 g. EtCO₂Et at 25.degree. gave 57.1 g. 6-Et deriv. (XI) of VII, m. 65-6.degree. (MeOH-H₂O), which (5.5 g.) oxidized in 150 ml. abs. EtOH with 9 g. m-ClC₆H₄CO₃H (XII) at 5.degree. gave, in addn. to 1 g. unreacted XI, 2 g. 6-Et deriv. of VIII, light yellow, m. 108.5-10.degree.; it gave mono- and di-HCl and BzOH salts. Similarly 43.5 g. 1,1-(3-oxapentamethylene)biquanide-HCl, MeONa, and EtOAc gave 25.7 g. 2-amino-4-methyl-6-morpholino-1,3,5-triazine, m. 184-5.degree., which oxidized with XII gave 1,2-dihydro-1-hydroxy-2-imino-6-methyl-4-morpholino-1,3,5-triazine, m. 254-5.degree.; it formed mono- and di-HCl and mono-H₃PO₄ salts. Similar oxidn. of 2-amino-4-methyl-6-piperidino-1,3,5-triazine gave 1,2-dihydro-1-hydroxy-2-imino-6-methyl-4-piperidino-1,3,5-triazine. 5-Cyclohexyl-1,1-ethylenebiquanide-HCl, prepd. by fusion of ethylenimine-HCl and 3-cyclohexyl-1-cyanoguanide, reacted with EtOAc and</p>				

NaOMe with the formation of 2-(1-aziridinyl)-4-cyclohexylamino-6-methyl-1,3,5-triazine and oxidized with XII gave 1,2-dihydro-1-hydroxy-4-(1-aziridinyl)-2-cyclohexylimino-6-methyl-1,3,5-triazine. VI (43.5 g.) reacted with PhCH₂CO₂Et and NaOMe to give 28.7 g. 2-amino-4-benzyl-6-diallylamino-1,3,5-triazine, m. 58-60.degree. (MeOH-H₂O), which oxidized with XII gave the 6-benzyl deriv. of VIII; it gave a pos. FeCl₃ test. VI, Et valerate, and MeONa gave the 6-Bu deriv. of VII, m. 32-4.degree., which oxidized gave the 6-Bu homolog of VIII, m. 82-5.degree.. VI, Me cyclohexanecarboxylate, and MeONa gave the 6-cyclohexyl deriv. of VII, m. 90-2.degree. (MeOH-H₂O) which on oxidn. gave the 6-cyclohexyl deriv. of VIII, m. 139-42.degree. (MeCN). VI (43.5 g.), 29.9 g. BzOMe, and MeONa gave the 6-Ph deriv. of VII, m. 82-4.degree. (MeOH), which oxidized gave the 6-Ph deriv. of VIII, yellow, m. 135-45.degree.. VI (65.3 g.), 30.1 g. Me acrylate, and MeONa 72 hrs. at 25.degree. gave 47 g. 2-amino-4-diallylamino-6-(2-methoxyethyl)-1,3,5-triazine, b0.2-0.7 144-60.degree., which oxidized gave light yellow 1,2-dihydro-1-hydroxy-4-diallylamino-2-imino-6-(2-methoxyethyl)-1,3,5-triazine, m. 132-4.degree. (MeCN). VI (43.5 g.), 22 g. Me crotonate, and MeONa gave the 6-(2-methoxypropyl) deriv. of VII, b0.25-0.4 145-7.degree., which oxidized gave the 6-(2-methoxypropyl) deriv. of VIII, viscous oil. VI (87 g.) was treated with MeOCH₂CH₂ONa (from 9.2 g. Na and 500 ml. MeOCH₂CH₂OH), the filtered soln. treated with 34.4 g. Me acrylate 63 hrs. at 25.degree., the concd. (in vacuo) soln. dild. with 2 l. H₂O and extd. with CH₂Cl₂, the dried ext. fractionally distd., and the fraction, b0.45-1 138-168.degree., crystd. to give 14.9 g. 6-vinyl deriv. of VII, m. 64-5.degree. (MeOH-H₂O), which oxidized with XII gave the 6-vinyl deriv. of VIII as a viscous oil. VI (43.5 g.), 22.5 g. PrCO₂Me, and MeONa 69 hrs. at 25.degree. gave 33.2 g. 6-Pr deriv. of VII, m. 50-2.degree. (MeOH-H₂O), which oxidized gave the 6-Pr deriv. of VIII, m. 88-91.degree. (MeCN). In the same way the 6-iso-Pr deriv. of VII, m. 49-51.degree. (EtOH-H₂O), and of VIII, m. 119-21.degree., were prepd. VI and AmCO₂Et gave the 6-Am deriv. of VII, b1 155-7.degree., and of VIII, yellow oil. 6-p-ClC₆H₄CH₂ deriv. of VII, prepd. from VI and p-ClC₆H₄CO₂Me, m. 87-9.degree., and of VIII, amorphous yellow powder, m. 65-80.degree.. VI (43.5 g.), 36.1 g. PhCH₂CH₂CO₂Me, and MeONa 45 hrs. at 25.degree. gave 37.8 g. 6-phenethyl deriv. of VI, viscous oil, b0.3 180-2.degree., which oxidized with XII gave the 6-phenethyl deriv. of VIII, m. 118-20.degree. (MeCN); it gave mono- and di-HCl and mono-H₂SO₄ salts. VI and Ph(CH₂)₃CO₂Me gave the 6-Ph(CH₂)₃ deriv. of VII, yellow, m. 57-60.degree., which oxidized gave the 6-Ph(CH₂)₃ deriv. of VIII, m. 91-3.degree. (MeCN). VI (52.2 g.) and 26 g. Me cyclopropenecarboxylate gave the 6-cyclopropyl deriv. of VII, m. 55-7.5.degree. (EtOH-H₂O), which oxidized gave the 6-cyclopropyl deriv. of VIII, m. 104-6.degree. (MeCN); its HCl, H₂SO₄, H₃PO₄, lactic, benzoic, and succinic acid salts were prepd. A soln. of 16.4 g. 2,4-dichloro-6-methyl-1,3,5-triazine (XIII) in 125 ml. Et₂O was added over 1.5 hrs. to 11.4 g. allylamine in 225 ml. Et₂O at 0-5.degree. and the soln. filtered and evapd. to give 11.9 g. 2-allylamino-4-chloro-6-methyl-1,3,5-triazine (XIV), m. 53-6.degree. (C₆H₁₄); it was treated with diallylamine in HCONMe, heated at 100.degree., and dild. with H₂O to give 2-allylamino-4-diallylamino-6-methyl-1,3,5-triazine (XV), m. 40-1.5.degree., which oxidized with XII gave 1,2-dihydro-1-hydroxy-2-allylimino-4-diallylamino-6-methyl-1,3,5-triazine (XVI), m. 78-80.degree. (C₆H₁₄) (sintering at 72.degree.). XIII and PhNH₂ gave the 2-anilino analog of XIV, m. 100-15.degree.; it reacted with diallylamine to give the 2-anilino analog of XV, yellow oil, b1.1 180-95.degree., which oxidized gave the 2-phenylimino analog of XVI, m. 103-5.degree. (C₆H₁₄). XIII and PhCH₂NH₂ gave the 2-benzyl-amino analog of XIV, light yellow, m. 98-100.degree. (C₆H₁₄), which was treated with diallylamine to give the

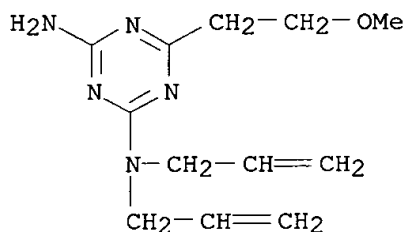
2-benzylamino analog (XVII) of XV, m. 67-9.degree.. XVII was oxidized with XII to give the 2-benzylimino analog of XVI, m. 84-6.degree. (sintering at 75.degree.) (C₆H₁₄). With these procedures 9 addnl. I and their intermediates are listed. The Me analog of X (400 mg.) in 5 ml. anhyd. Et₂O was treated with 3 drops Ac₂O to give 450 mg. 1,2-dihydro-1-hydroxy-2-acetylimino-4-diallylamino-6-methyl-1,3,5-triazine-AcOH, m. 91-2.degree., which with Et₃N gave the free base. With AcCl in lieu of Ac₂O the HCl salt was formed. With this method but using different acid anhydrides 9 addnl. I are prepd. With 18 other triazines in lieu of X 18 addnl. 1,2-dihydro-1-hydroxy-2,4-substituted-2-acetylimino-1,3,5-triazines were formed. Using 1 ml. Ac₂O in 15 ml. Et₂O in lieu of 3 drops and refluxing the mixt. 4 hrs. gave 1,2-dihydro-1-acetoxy-2-acetylimino-4-diallylamino-6-methyl-1,3,5-triazine. With other acid anhydrides 5 other diacylated I were prepd. The uv absorption bands of some of the compds. are given.

IT **5122-68-9P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 5122-68-9 CAPLUS

CN s-Triazine, 2-amino-4-(diallylamino)-6-(2-methoxyethyl)- (7CI, 8CI) (CA INDEX NAME)



L14 ANSWER 16 OF 38 CAPLUS COPYRIGHT 2002 ACS

AN 1996:113265 CAPLUS

DN 124:146146

TI preparation of thiazolyliminosulfonylurea derivatives as herbicides

IN Makino, Kenji; Suzuki, Hideaki; Nagaoka, Takeshi; Niki, Toshio; Hamada, Toshimasa; Kusuoka, Yoshuki; Nawamaki, Tsutomu; Watanabe, Shigeomi; Ito, Yoichi; Et, Al.

PA Nissan Chemical Ind Ltd, Japan

SO Jpn. Kokai Tokkyo Koho, 48 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 07252253	A2	19951003	JP 1995-4248	19950113
PRAI	JP 1994-7703		19940127		

OS MARPAT 124:146146

AB The title compds. [I; R1 = alkyl, alkenyl, alkynyl, etc.; R2 = (substituted) pyrimidinyl, triazinyl, etc., bond a = satd., unsatd.] are prepd. ClSO₂NCO was added dropwise to a suspension of triazine deriv. II in THF with stirring at room temp., followed by a suspension of III in THF and Et₃N, and the mixt. was stirred at room temp. to give I [R1 = 3-chloroallyloxy, R2 = 4-methoxy-6-(methoxymethyl)triazin-2-yl, a = satd.], which killed >90% barnyard grass and Setaria viridis at 6.3 g/are.

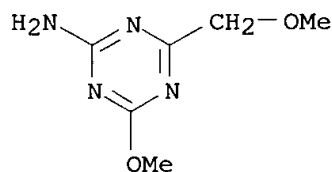
IT 125069-39-8, 2-Amino-4-methoxy-6-(methoxymethyl)triazine

RL: RCT (Reactant)

(prepn. of thiazolyliminosulfonylurea derivs. as herbicides)

RN 125069-39-8 CAPLUS

CN 1,3,5-Triazin-2-amine, 4-methoxy-6-(methoxymethyl)- (9CI) (CA INDEX NAME)



L14 ANSWER 21 OF 38 CAPLUS COPYRIGHT 2002 ACS
 AN 1985:220904 CAPLUS
 DN 102:220904
 TI Heterocyclic substituted sulfonylureas
 IN Willms, Lothar; Humburg, Gerhard; Bauer, Klaus; Bieringer, Hermann;
 Buerstell, Helmut
 PA Hoechst A.-G. , Fed. Rep. Ger.
 SO Ger. Offen., 29 pp.
 CODEN: GWXXBX
 DT Patent
 LA German
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 3324800	A1	19850117	DE 1983-3324800	19830709
	EP 134477	A1	19850320	EP 1984-107831	19840705
	R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE				
	DK 8403350	A	19850110	DK 1984-3350	19840706
	DD 220217	A5	19850327	DD 1984-265012	19840706
	ES 534113	A1	19850401	ES 1984-534113	19840706
	BR 8403369	A	19850618	BR 1984-3369	19840706
	JP 60038370	A2	19850227	JP 1984-139790	19840707
	ZA 8405216	A	19850227	ZA 1984-5216	19840708
	AU 8430433	A1	19850110	AU 1984-30433	19840709
PRAI	DE 1983-3324800		19830709		

OS CASREACT 102:220904

AB Pyrimidinyl- and triazinyl(phenylsulfonyl)ureas I [R = (un)substituted Ph; R1, R2 = H, alkyl; R3 = H, alkoxy, alkylthio, CH2:CHCH2O, HC.tplbond.CHCH2O, amino, (un)substituted alkyl; R4, R5 = H, halo, (un)substituted alkyl; R6 = alkyl, alkenyl, PhCH2; X = CH2, N; n = 1-3; m = 0-2] were prepd. Thus, H2NC(:NH2)N:C(OMe)NH2.HCl in MeOH was treated with Na and MeSCH2CO2Et to give 52% 4-methoxy-6-[(methylthio)methyl]-1,3,5-triazin-2-amine. This was stirred 18 h at room temp. in CH2Cl2 with 2-ClC6H4SO2NCO to give 79.5% triazinylurea II. In preemergence tests 2.5 kg II/ha gave 80-100% control of, e.g., Stellaria media.

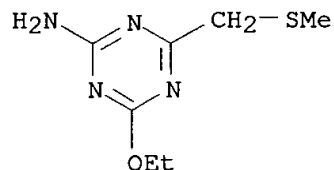
IT **96601-55-7 96601-56-8 96602-44-7**

RL: RCT (Reactant)

(condensation of, with benzenesulfonyl isocyanate deriv.)

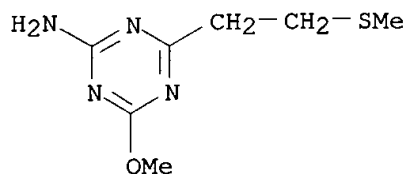
RN 96601-55-7 CAPLUS

CN 1,3,5-Triazin-2-amine, 4-ethoxy-6-[(methylthio)methyl]- (9CI) (CA INDEX NAME)



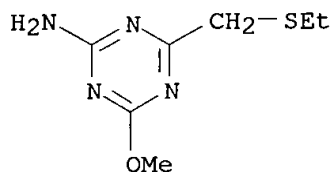
RN 96601-56-8 CAPLUS

CN 1,3,5-Triazin-2-amine, 4-methoxy-6-[2-(methylthio)ethyl]- (9CI) (CA INDEX NAME)



RN 96602-44-7 CAPLUS

CN 1,3,5-Triazin-2-amine, 4-[(ethylthio)methyl]-6-methoxy- (9CI) (CA INDEX NAME)

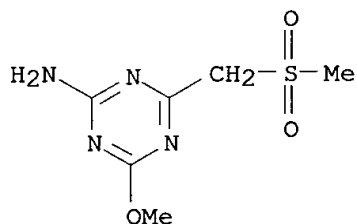


IT **96602-43-6P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation of, with benzenesulfonyl isocyanates)

RN 96602-43-6 CAPLUS

CN 1,3,5-Triazin-2-amine, 4-methoxy-6-[(methylsulfonyl)methyl]- (9CI) (CA INDEX NAME)

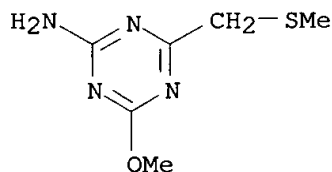


IT **96602-42-5P**

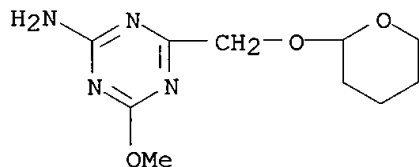
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn., oxidn., and condensation of, with benzenesulfonyl isocyanates)

RN 96602-42-5 CAPLUS

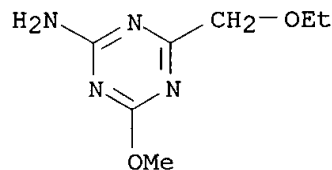
CN 1,3,5-Triazin-2-amine, 4-methoxy-6-[(methylthio)methyl]- (9CI) (CA INDEX NAME)



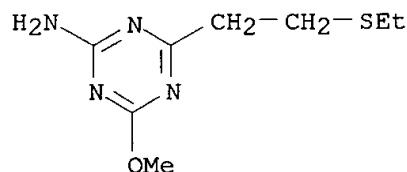
L14 ANSWER 22 OF 38 CAPLUS COPYRIGHT 2002 ACS
AN 1984:586001 CAPLUS
DN 101:186001
TI Metabolism of chlorsulfuron by tolerant broadleaves
AU Hutchison, J. M.; Shapiro, R.; Sweetser, P. B.
CS E. I. du Pont de Nemours and Co., Inc., Wilmington, DE, 19898, USA
SO Pestic. Biochem. Physiol. (1984), 22(2), 243-7
CODEN: PCBPBS; ISSN: 0048-3575
DT Journal
LA English
AB The ability of flax (*Linum usitatissimum*) and black nightshade (*Solanum nigrum*) to metabolize chlorsulfuron [64902-72-3] was studied to det. if metab. contributes to tolerance, and to identify any metabolites produced. Plant leaves were treated with [¹⁴C]chlorsulfuron for a 24-h period. The metabolites were extd., sepd. by high-performance liq. chromatog., and characterized. Mass spectral anal. and independent synthesis confirmed a major metabolite (B-1) as 2-chloro-N-[[4-(hydroxymethyl)-6-methoxy-1,3,5-triazin-2-yl]aminocarboxyl]benzenesulfonamide [87644-23-3]. A second major metabolite (B) was a carbohydrate conjugate of B-1. Plants were more tolerant to B-1 applications than to chlorsulfuron. Thus, metab. may be the basis of selectivity to chlorsulfuron for tolerant broadleaf plants as well as for grasses.
IT **92533-23-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, with chlorobenzenesulfonyl isocyanate)
RN 92533-23-8 CAPLUS
CN 1,3,5-Triazin-2-amine, 4-methoxy-6-[[4-(tetrahydro-2H-pyran-2-yl)oxy]methyl]-
(9CI) (CA INDEX NAME)



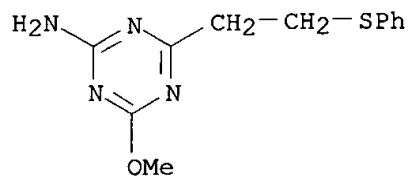
L14 ANSWER 30 OF 38 CAPLUS COPYRIGHT 2002 ACS
 AN 1975:564133 CAPLUS
 DN 83:164133
 TI Heterocyclic compounds. I. Syntheses of 1,3,5-triazine derivatives and their pharmacological activities. 1
 AU Tsujikawa, Teruaki; Takei, Saburo; Tsushima, Susumu; Tsuda, Takashi; Tsukamura, Kazuo; Sirakawa, Kenzo; Chiba, Sukehiro; Nagawa, Yuji; Yui, Tohoru
 CS Cent. Res. Div., Takeda Chem. Ind., Ltd., Osaka, Japan
 SO Yakugaku Zasshi (1975), 95(5), 499-511
 CODEN: YKKZAJ
 DT Journal
 LA Japanese
 AB 6-Alkoxy-2-alkyl-4-amino-1,3,5-triazines and related compds. were synthesized and their pharmacol. activities were examd. Main characteristics of these compds. after their intraperitoneal administration were divided into two categories, sedation and convulsion. The sedative effect was parallel to potentiation of barbiturate hypnosis. No clear relationship was found between anticonvulsant and sedative effects. In many cases, the compds. with phenylpiperazinyl group produced fall in blood pressure. This hypotension seems to be due at least in part, to central action of the compd.
 IT **5270-22-4P 5270-25-7P 5270-28-0P**
5375-81-5P
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (prepn. and pharmacol. activity of)
 RN 5270-22-4 CAPLUS
 CN 1,3,5-Triazin-2-amine, 4-(ethoxymethyl)-6-methoxy- (9CI) (CA INDEX NAME)



RN 5270-25-7 CAPLUS
 CN 1,3,5-Triazin-2-amine, 4-[2-(ethylthio)ethyl]-6-methoxy- (9CI) (CA INDEX NAME)

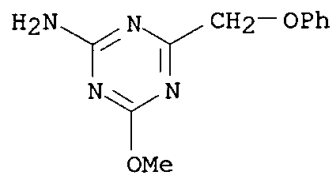


RN 5270-28-0 CAPLUS
 CN 1,3,5-Triazin-2-amine, 4-methoxy-6-[2-(phenylthio)ethyl]- (9CI) (CA INDEX NAME)



RN 5375-81-5 CAPLUS

CN 1,3,5-Triazin-2-amine, 4-methoxy-6-(phenoxymethyl)- (9CI) (CA INDEX NAME)

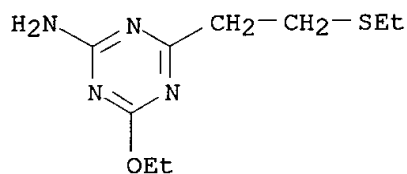


IT **56968-42-4P 56968-49-1P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

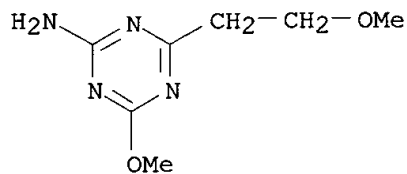
RN 56968-42-4 CAPLUS

CN 1,3,5-Triazin-2-amine, 4-ethoxy-6-[2-(ethylthio)ethyl]- (9CI) (CA INDEX NAME)



RN 56968-49-1 CAPLUS

CN 1,3,5-Triazin-2-amine, 4-methoxy-6-(2-methoxyethyl)- (9CI) (CA INDEX NAME)



L14 ANSWER 36 OF 38 CAPLUS COPYRIGHT 2002 ACS

AN 1968:459209 CAPLUS

DN 69:59209

TI Antitumor substances. VII. Reaction of N-amidino-O-alkylisourea with some carboxylic esters

AU Hayashi, Seigoro; Furukawa, Mitsuru; Yamamoto, Junko; Nishizima, Yoko

CS Fac. Pharm. Sci., Kumamoto Univ., Kumamoto, Japan

SO Chem. Pharm. Bull. (Tokyo) (1968), 16(3), 474-9

CODEN: CPBTAL

DT Journal

LA English

AB The reaction of N-amidino-O-alkylisourea with some carboxylic esters was studied. Condensation with diethyl oxalate in alc. gave alkyl 4-amino-6-alkoxy-s-triazine-2-carboxylate through formation of a five-membered-ring intermediate. Alkyl 4-amino-6-alkoxy-s-triazine-2-carboxylate was easily converted into the corresponding amide with a variety of amines. Condensation with ethyl acetoacetate gave 6-methyl-2-alkoxyamidino-4-pyrimidinol and 4-amino-2-alkoxy-6-acetomethyl-s-triazine. Condensation with ethyl cyanoacetate afforded only 4-amino-2-alkoxy-6-cyanomethyl-s-triazine, but not any expected pyrimidinol. Condensation with ethyl chloroacetate gave 4-amino-2-alkoxy-6-chloromethyl-s-triazine, which was converted into 4-amino-2-alkoxy-6-substituted amino-s-triazine with a variety of amines.

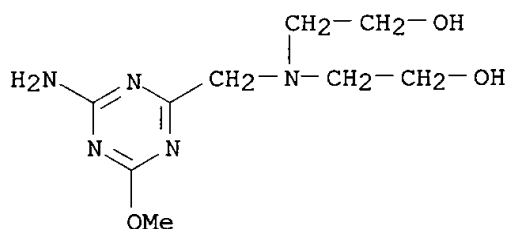
IT 19840-00-7P 19840-01-8P 19840-06-3P

19840-07-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

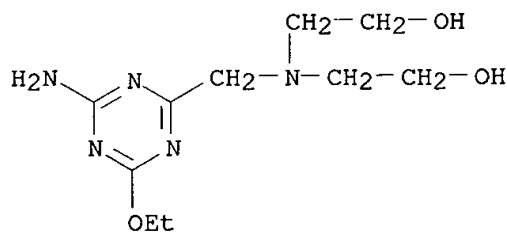
RN 19840-00-7 CAPLUS

CN Ethanol, 2,2'-[[(4-amino-6-methoxy-s-triazin-2-yl)methyl]imino]di- (8CI)
(CA INDEX NAME)



RN 19840-01-8 CAPLUS

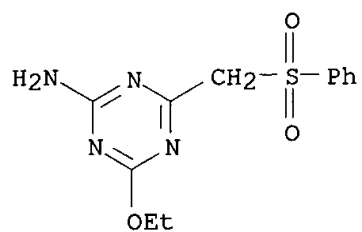
CN Ethanol, 2,2'-[[(4-amino-6-ethoxy-s-triazin-2-yl)methyl]imino]di- (8CI)
(CA INDEX NAME)



RN 19840-06-3 CAPLUS

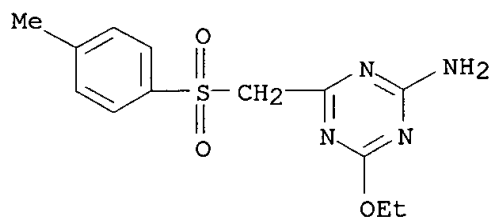
10/005,064

CN s-Triazine, 2-amino-4-ethoxy-6-[(phenylsulfonyl)methyl]- (8CI) (CA INDEX NAME)



RN 19840-07-4 CAPLUS

CN s-Triazine, 2-amino-4-ethoxy-6-[(p-tolylsulfonyl)methyl]- (8CI) (CA INDEX NAME)



L15 ANSWER 1 OF 11 CAOLD COPYRIGHT 2002 ACS

AN CA64:12702d CAOLD

TI 2-amino-4-alkoxy-1,3,5-triazines

AU Tsuda, Takashi; Takei, S.; Tsujikawa, T.

DT Patent

TI 2-amino-4-alkoxy-S-triazines

PA Takeda Chemical Industries, Ltd.

DT Patent

PATENT NO.	KIND	DATE
JP 66001115		1966
NL 6504702		
BE 662676		
DE 1212545		
FR 1432109		
GB 1030587		
IT 5270-22-4	5270-25-7	5270-28-0
5375-81-5		

PI JP 66001115

1966

PI NL 6504702

BE 662676

DE 1212545

FR 1432109

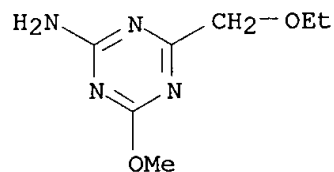
GB 1030587

IT 5270-22-4 5270-25-7 5270-28-0

5375-81-5

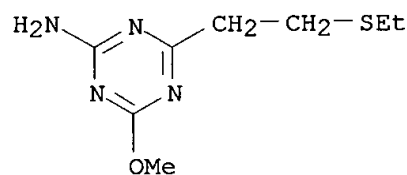
RN 5270-22-4 CAOLD

CN 1,3,5-Triazin-2-amine, 4-(ethoxymethyl)-6-methoxy- (9CI) (CA INDEX NAME)



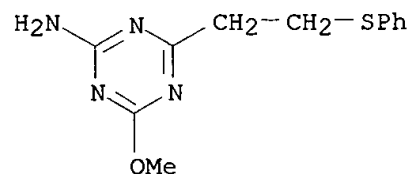
RN 5270-25-7 CAOLD

CN 1,3,5-Triazin-2-amine, 4-[2-(ethylthio)ethyl]-6-methoxy- (9CI) (CA INDEX NAME)



RN 5270-28-0 CAOLD

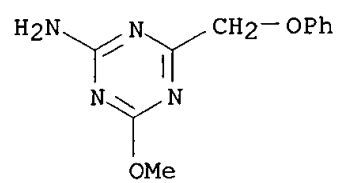
CN 1,3,5-Triazin-2-amine, 4-methoxy-6-[2-(phenylthio)ethyl]- (9CI) (CA INDEX NAME)



RN 5375-81-5 CAOLD

CN 1,3,5-Triazin-2-amine, 4-methoxy-6-(phoxymethyl)- (9CI) (CA INDEX NAME)

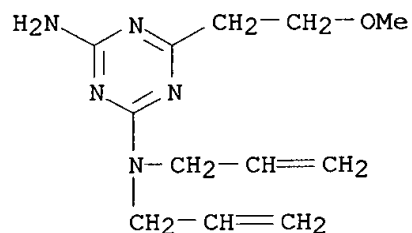
10/005,064



L15 ANSWER 2 OF 11 CAOLD COPYRIGHT 2002 ACS
 AN CA64:5117f CAOLD
 TI 1,2-dihydro-2-imino-1,3,5-triazine 1-ether derivs.
 PA Upjohn Co.
 DT Patent

PATENT NO.	KIND	DATE
NL 6501753		
US 3270018		1966

 IT **5122-68-9**
 RN 5122-68-9 CAOLD
 CN s-Triazine, 2-amino-4-(diallylamino)-6-(2-methoxyethyl)- (7CI, 8CI) (CA INDEX NAME)



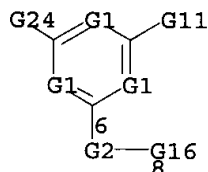
L31 ANSWER 1 OF 8 MARPAT COPYRIGHT 2002 ACS
 AN 136:263168 MARPAT
 TI Preparation of substituted heterocyclic aryl-alkyl-aryl compounds as
 thrombin inhibitors
 IN Isaacs, Richard C.; Williams, Peter D.; Lyle, Terry A.; Staas, Donnette
 D.; Savage, Kelly L.
 PA Merck & Co., Inc., USA
 SO PCT Int. Appl., 91 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002022584	A1	20020321	WO 2001-US28791	20010911
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRAI US 2000-231656P 20000911

AB Title compds. I [u, v, w = CH, N; X = O, SOO-2, NH, alkenyl, C:O, C:ONH, C:OO, alkyl, CH₂NH, CH₂O, CF₂; Y = (CH₂)₀₋₁(CR₄R₅)(CH₂)₀₋₁; Z = O, SO-2, C:O, amino, CF₂, bond; R₁ = H, alkyl(CN), C:O, (CH₂)₀₋₁-carboxy, CF₃, alkoxy, halo, SOO-2, amino; R₂ = (un)substituted Ph, 5-6-membered heterocycle; R₃ = Ph, (un)substituted ring system, 5-6-membered heterocycle; R₄₋₅ = H, alkyl; R₆, R₈ = halo, alkylamino, heterocycle] were prepd. Examples include data for over 20 compds., 3 solid oral dosage formulations and an in-vitro assay for protease detn. for example compds. For instance, 2'-isopropyl-5-methylbiphenyl-3-ol (prepd. in 3 steps from 2-isopropylphenyl iodide) was reacted with (S)-2-(pyridin-4-ylamino)propan-1-ol to give II isolated as the trifluoroacetate. Example compds. exhibited inhibitory activity against human thrombin, K_i < 24 nM. I are useful in the treatment of blood coagulation and cardiovascular disorders.

MSTR 1



G1 = N
 G5 = CH₂
 G6 = O
 G14 = S
 G15 = alkyl<(1-4)>
 G24 = Hy<EC (1-2) Q (0-) N (0-) O (0-) S (0) OTHERQ,
 AR (0), BD (ALL) SE, RC (1), RS (1) E6>
 (SO (1-3) alkyl<(1-8)>)
 G29 = CH₂

MPL: claim 1
 NTE: substitution is restricted
 NTE: or pharmaceutically acceptable salts

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 2 OF 8 MARPAT COPYRIGHT 2002 ACS

AN 135:33374 MARPAT

TI Nitrosulfo benzamides, processes for their preparation, and their use in the production of sulfonylurea herbicides

IN Ford, Mark James; Vermehren, Jan

PA Aventis Cropscience G.m.b.H., Germany

SO PCT Int. Appl., 59 pp.

CODEN: PIXXD2

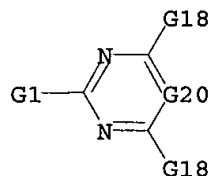
DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001042226	A1	20010614	WO 2000-EP11501	20001118
	W: AE, AG, AL, AM, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CN, CR, CU, CZ, DM, DZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KP, KR, KZ, LC, LK, LR, LT, LV, MA, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TT, UA, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 2001020092	A1	20010906	US 2000-732006	20001207
PRAI	DE 1999-19959291		19991209		
AB	The invention relates to nitrosulfo benzamides I [wherein R ₁ , R ₂ = (un)substituted C ₁ -10 (preferably C ₁ -6) hydrocarbon radical; or NR ₁ R ₂ = (un)substituted 3- to 8-membered heterocyclic ring optionally contg. 1 or 2 further N/O/S ring heteroatoms; Q = H or cation]. I can be used advantageously for the prepn. of sulfonylurea herbicides, and their precursors such as sulfonyl chlorides or sulfonamides. For instance, reaction of 4-nitro-2-sulfo benzoic acid dipotassium salt with phosgene in PhMe in the presence of DMF and pyridine, followed by removal of excess phosgene and then addn. of dimethylamine, gave title compd. I [R ₁ = R ₂ = Me, Q = K] in 90% yield and 80% purity (isolated). Alternatively, prepn. and further treatment of the above product in situ with phosgene and then with ammonia gave N,N-dimethyl-2-aminosulfonyl-4-nitrobenzamide in 81% yield and 93.4% purity. When this sulfonamide intermediate was treated yet again with phosgene and then with 2-amino-4,6-dimethoxypyrimidine, the sulfonylurea deriv. II [X = NO ₂] was obtained in 58% yield and 87% purity. Hydrogenation of the latter in formic acid in the presence of Na molybdate gave II [X = NHCHO], i.e. foramsulfuron, in 83.6% yield and 95.5% purity. Foramsulfuron was also prepd. using I via another invention route with earlier introduction of the formamide moiety.				

MSTR 5



G1 = NH2
 G4 = S
 G5 = alkyl<(1-6)> (SO (1-) G19)
 G18 = alkyl<(1-6)> (SO (1-) G19)
 G19 = alkoxy<(1-4)>
 G20 = N
 MPL: claim 18

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 3 OF 8 MARPAT COPYRIGHT 2002 ACS

AN 130:95383 MARPAT

TI Preparation of aryne intermediates useful in herbicide manufg.

IN Harrington, Philip M.; Kremer, Kenneth A. M.

PA American Cyanamid Company, USA

SO U.S., 9 pp.

CODEN: USXXAM

DT Patent

LA English

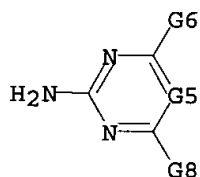
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5856576	A	19990105	US 1998-15817	19980129
	CN 1187485	A	19980715	CN 1998-103947	19980106
PRAI	US 1998-15817		19980129		

OS CASREACT 130:95383

AB The title compds. [I; R = H, CN, F, etc.; X = NO2, NR1R2; Z = OH, Br, Cl, OSO2R3; R1, R2 = H, CHO, Ac, etc.; R3 = C1-6 alkyl, C1-6 haloalkyl, (un)substituted Ph], useful intermediates in the manuf. of herbicidal compds., were prep'd. by palladium catalyzed coupling of an o-halonitrobenzene or o-haloaniline with 3-butyne-1-ol.

MSTR 8



G3 = alkoxy<(1-3)>
 G5 = N
 G6 = alkylthio<(1-4)> (SO (1-) G3)
 G8 = alkyl<(1-4)> (SO (1-) G3)
 MPL: claim 17

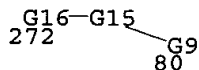
RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

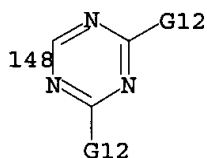
L31 ANSWER 4 OF 8 MARPAT COPYRIGHT 2002 ACS
 AN 129:275833 MARPAT
 TI Combinatorial synthesis and screening of .alpha.-ketoamide-derivative
 cysteine protease inhibitors
 IN Blandino, Carmen M.; Coffen, David L.; Chipman, Stewart D.; Cheng, Hong
 PA Argule, Inc., USA
 SO PCT Int. Appl., 71 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9846559	A1	19981022	WO 1998-US7747	19980416
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9871290	A1	19981111	AU 1998-71290	19980416
	EP 975584	A1	20000202	EP 1998-918344	19980416
	R: CH, DE, DK, FR, GB, IT, LI, NL, SE				
PRAI	US 1997-843584		19970416		
	WO 1998-US7747		19980416		
AB	Via combinatorial synthesis, about 38,000 .alpha.-ketoamide derivs. were prepd. and the arrays screened, from which 6 compds. were isolated which had a high inhibitory activity against three cysteine proteases: cruzain, papain, and cathepsin B; these title compds. may be useful in the treatment of diseases (e.g., Chagas' disease) assocd. with these proteases. Thus, Me 2-(2-benzothienyl)-2-oxoethanoate was amidated with 4-aminobenzyl amine, the intermediate isolated and reacted with benzyl isothiocyanate, producing ther 2-benzothienyl .alpha.-ketoamide I which demonstrated an IC50 for cruzain of 2.2 .mu.M and 3.3 .mu.M for cathepsin B.				

MSTR 2



G2 = NH
 G9 = 148



G10 = S
 G12 = alkyl (SO (1-) G3)
 G17 = alkyl (SO (1-) G3)
 G18 = O
 G19 = acyl
 MPL: claim 17
 NTE: also incorporates claim 53

L31 ANSWER 5 OF 8 MARPAT COPYRIGHT 2002 ACS

AN 127:262707 MARPAT

TI Substituted aryl sulfonyl(thio)ureas used as herbicides

IN Gesing, Ernst Rudolf F.; Kirsten, Rolf; Kluth, Joachim; Muller, Klaus-Helmut; Drewes, Mark Wilhelm; Jansen, Johannes Rudolf; Philipp, Ulrich; Riebel, Hans-Jochem; Schallner, Otto; Dollinger, Markus; Santel, Hans-Joachim

PA Bayer A.-G., Germany; Gesing, Ernst Rudolf F.; Kirsten, Rolf; Kluth, Joachim; Muller, Klaus-Helmut; Drewes, Mark Wilhelm; Jansen, Johannes Rudolf; Philipp, Ulrich; Riebel, Hans-Jochem; et al.

SO PCT Int. Appl., 54 pp.

CODEN: PIXXD2

DT Patent

LA German

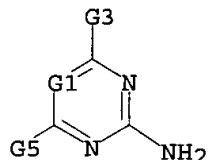
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9732861	A1	19970912	WO 1997-EP798	19970220
	W: AU, BB, BG, BR, BY, CA, CN, CZ, HU, IL, JP, KR, KZ, LK, MX, NO, NZ, PL, RO, RU, SK, TR, UA, US				
	RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	DE 19608445	A1	19970911	DE 1996-19608445	19960305
	CA 2248068	AA	19970912	CA 1997-2248068	19970220
	AU 9720917	A1	19970922	AU 1997-20917	19970220
	AU 712363	B2	19991104		
	EP 885200	A1	19981223	EP 1997-906098	19970220
	R: DE, DK, ES, FR, GB, IT				
	CN 1212686	A	19990331	CN 1997-192820	19970220
	BR 9707917	A	19990727	BR 1997-7917	19970220
PRAI	DE 1996-19608445		19960305		
	WO 1997-EP798		19970220		

AB The invention relates to novel substituted arylsulfonyl(thio)ureas I and their salts [wherein A = N or CH; Q = O or S; R1 = H, halo, or (un)substituted alkyl, alkoxy, alkylthio, alkylamino, dialkylamino, cycloalkyl, cycloalkyloxy, or heterocyclyloxy; R2 = H, halo, or (un)substituted alkyl, alkoxy, alkylthio, alkylamino, dialkylamino, cycloalkyl, cycloalkyloxy, or heterocyclyloxy; R3 = H or (un)substituted alkyl; R4 = (un)substituted alkyl, alkoxy, alkenyl, alkynyl, alkenyloxy, alkynyloxy, cycloalkyl, cycloalkyloxy, or cycloalkylalkyl; and R5 = H, formyl, or (un)substituted alkyl, alkylcarbonyl, alkoxycarbonyl, alkylsulfonyl, alkenyl, alkynyl, cycloalkyl, cycloalkylcarbonyl, cycloalkylsulfonyl, or heterocyclyl; except for the compd. N-(4,6-dimethylpyrimidin-2-yl)-N'-[[2-(1,1,2,2-tetrafluoroethoxy)-6-methylphenyl]sulfonyl]urea]. Also disclosed are a process for producing the novel compds., and their use as herbicides. For example, condensation of 2-methoxy-6-methylbenzenesulfonamide with 2-[N,N-bis(phenoxycarbonyl)amino]-4,6-dimethoxy-1,3,5-triazine in MeCN in the presence of KOBu-tert, followed by stirring with 1N aq. HCl and CH2Cl2, gave 55% title compd. II. At 30 g/ha preemergence, II gave complete kill of 6 test plants: Alopecurus, Lolium, Sorghum, Amaranthus, Chenopodium,

and Stellaria.

MSTR 2



G1 = N
 G3 = alkylthio (SO (1-) G11)
 G5 = alkyl (SO (1-) G11)
 G11 = alkoxy<(1-4)>
 MPL: claim 4

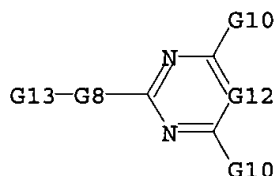
L31 ANSWER 6 OF 8 MARPAT COPYRIGHT 2002 ACS
 AN 124:146187 MARPAT
 TI Preparation of N-[acylamino(carbamoyl)phenylsulfonyl]-N'-pyrimidinylureas
 as herbicides and plant growth regulators
 IN Schnabel, Gerhard; Willms, Lothar; Bauer, Klaus; Bieringer, Hermann
 PA Hoechst Schering Agrevo GmbH, Germany
 SO Ger. Offen., 27 pp.
 CODEN: GWXXBX
 DT Patent
 LA German
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 4415049	A1	19951102	DE 1994-4415049	19940429
	CA 2189044	AA	19951109	CA 1995-2189044	19950412
	WO 9529899	A1	19951109	WO 1995-EP1344	19950412
	W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TT, UA, UZ, VN				
	RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9523441	A1	19951129	AU 1995-23441	19950412
	EP 757679	A1	19970212	EP 1995-917311	19950412
	EP 757679	B1	19981021		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL				
	CN 1147252	A	19970409	CN 1995-192788	19950412
	CN 1066140	B	20010523		
	HU 76144	A2	19970728	HU 1996-2966	19950412
	BR 9507562	A	19970805	BR 1995-7562	19950412
	JP 09512538	T2	19971216	JP 1995-527953	19950412
	AT 172456	E	19981115	AT 1995-917311	19950412
	ES 2125012	T3	19990216	ES 1995-917311	19950412
	RO 114894	B3	19990830	RO 1996-1949	19950412
	ZA 9503436	A	19960117	ZA 1995-3436	19950428
	US 5922646	A	19990713	US 1997-906238	19970804
	CN 1295067	A	20010516	CN 2000-108955	20000524
PRAI	DE 1994-4415049		19940429		
	WO 1995-EP1344		19950412		

US 1995-429933 19950427

AB Title compds. [I; R = halo, alkyl, alkoxy; R1 = H, (un)substituted hydrocarbyl(oxy); R2 = H, (un)substituted hydrocarbyl; NR1R2 = heterocyclyl; R3 = acyl; R4 = H, aliph. hydrocarbyl; W1,W2 = O, S; X,Y = halo, alkyl, alkoxy, etc.; Z = CH or N; n = 0-3] were prepd. as herbicides and plant growth regulators (no data). Thus, 2,4-(H2N)(O2N)C6H3CO2H was converted in 7 steps 2-dimethylaminocarbonyl-5-methoxycarbonylaminobenzenesulfonamide which was condensed with 4,6-dimethoxy-2-(phenoxycarbonylamino)pyrimidine to give title compd. II.

MSTR 3



G8 = NH
 G10 = alkyl<(1-6)> (SO (1-) G11) /
 alkylthio<(1-6)> (SO (1-) G11)
 G11 = alkoxy<(1-4)>
 G12 = N
 MPL: claim 5

L31 ANSWER 7 OF 8 MARPAT COPYRIGHT 2002 ACS

AN 121:9426 MARPAT

TI Preparation of thienylsulfonylureidoazine herbicides.

IN Gesing, Ernst R. F.; Santel, Hans Joachim; Luerksen, Klaus; Schmidt, Robert Rudolf

PA Bayer A.-G., Germany

SO Ger. Offen., 15 pp.

CODEN: GWXXBX

DT Patent

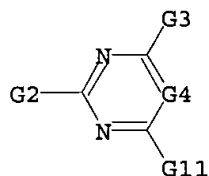
LA German

FAN.CNT 1

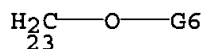
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 4232417	A1	19940331	DE 1992-4232417	19920928
	EP 590416	A1	19940406	EP 1993-114858	19930915
	R: BE, CH, DE, FR, GB, IT, LI, NL				
	US 5430006	A	19950704	US 1993-124919	19930921
	JP 06199848	A2	19940719	JP 1993-257547	19930922
	US 5508441	A	19960416	US 1995-412432	19950329
PRAI	DE 1992-4232417		19920928		
	US 1993-124919		19930921		

AB Title compds. [I; R1 = Et, Pr; R2 = H, Me; X, Y = H, OH, amino, cyano, halo, alkyl, cycloalkyl, haloalkyl, alkoxyalkyl, alkoxy, haloalkoxy, alkoxyalkoxy, alkylthio, alkylamino, dialkylamino; Z = N, CH, CR3; R3 = halo], were prepd. as herbicides (no data). Thus, Ph chloroformate was added to a mixt. of 2-ethoxycarbonylthiophene-3-sulfonamide and Et3N in MeCN; after 30 min. methanesulfonic acid and 2-amino-4-methoxy-6-methyl-s-triazine were added followed by 30 min. reflux to give title compd. II. Several I were said to show very strong herbicidal activity and good compatibility with crop plants.

MSTR 5



G2 = NH₂
 G3 = 23



G4 = N
 G6 = Me
 G11 = alkylthio<(1-4)>
 MPL: claim 4

L31 ANSWER 8 OF 8 MARPAT COPYRIGHT 2002 ACS

AN 115:183348 MARPAT

TI Preparation of (pyridylsulfonyl)ureas as herbicides and plant growth regulators

IN Kehne, Heinz; Willms, Lothar; Ort, Oswald; Bauer, Klaus; Bieringer, Hermann

PA Hoechst A.-G., Fed. Rep. Ger.

SO PCT Int. Appl., 74 pp.

CODEN: PIXXD2

DT Patent

LA German

FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9110660	A1	19910725	WO 1990-EP2308	19901224
	W: AT, AU, BB, BG, BR, CA, CH, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MC, MG, MW, NL, NO, RO, SD, SE, SU, US				
	RW: AT, BE, BF, BJ, CF, CG, CH, CM, DE, DK, ES, FR, GA, GB, GR, IT, LU, ML, MR, NL, SE, SN, TD, TG				
	DE 4000503	A1	19910711	DE 1990-4000503	19900110
	AU 9170484	A1	19910805	AU 1991-70484	19901224
	AU 648058	B2	19940414		
	EP 510032	A1	19921028	EP 1991-901751	19901224
	EP 510032	B1	19961113		
	R: BE, CH, DE, ES, FR, GB, GR, IT, LI, NL				
	BR 9007976	A	19921110	BR 1990-7976	19901224
	HU 61746	A2	19930301	HU 1992-2275	19901224
	JP 05503514	T2	19930610	JP 1991-502068	19901224
	US 5635451	A	19970603	US 1992-859513	19920608
	US 5494886	A	19960227	US 1994-337139	19941110
PRAI	DE 1990-4000503		19900110		
	DE 1990-4030577		19900927		
	DE 1990-4030557		19900927		
	WO 1990-EP2308		19901224		

US 1992-859513 19920608

US 1993-108896 19930818

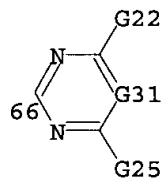
AB The title compds. [I; R = SO₂NHC(:W)NR₃A; A = (un)substituted pyrimidinyl, triazinyl, etc.; R₁ = iodo, NR₆R₇, OSO₂NR₄R₅; R₂ = H, (halo)alkyl, halo, NO₂, cyano, etc.; R₃ = H, Me; R₄ = H, alkyl, alkenyl, alkynyl, alkoxy; R₅ = H, alkyl, alkenyl, alkynyl; R₄R₅ = (CH₂)₄₋₅, CH₂CH₂OCH₂CH₂; R₆ = H, (halo)alkenyl, (un)substituted alkyl, alkylsulfonyl, PhSO₂, etc.; R₇ = (un)substituted alkylsulfonyl, PhSO₂; R₆R₇ = (CH₂)_mSO₂; W = O, S; m = 3, 4; n = 0, 1] were prep'd. Thus, PhCH₂SH was condensed with 2-fluoro-3-iodopyridine and the product converted in 2 steps to I (R = SO₂NHR₁₀, R₁ = iodo, R₂ = H) (II; R₁₀ = H) which was condensed with R₁₂NHCO₂Ph (R₁₂ = pyrimidinyl group Q) to give II (R₁₀ = CONHQ). The latter gave complete control of 6 weeds, e.g., Avena sativa, at 0.3 kg/ha preemergent.

MSTR 5

H—G7—G21

G7 = NH

G21 = 66



G23 = alkylene<(1-3)>

G24 = alkoxy<(1-3)>

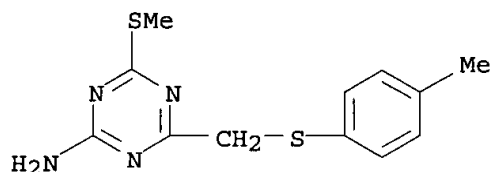
G25 = alkylthio<(1-3)> (SO (1-) G26)

G31 = N

DER: or salts

MPL: claim 5

L36 ANSWER 1 OF 5 CHEMCATS COPYRIGHT 2002 ACS
 Accession No. (AN): 1998:635165 CHEMCATS
 Catalog Name (CO): Maybridge HTS
 Publication Date (PD): 6 Feb 2002
 Order Number (ON): SPB 06116
 Chemical Name (CN): 4-[[[(4-methylphenyl)thio]methyl]-6-(methylthio)-1,3,5-triazin-2-amine
 CAS Registry No. (RN): **265314-66-7**
 Supplementary Term (ST): CHEMICAL LIBRARY
 Structure :

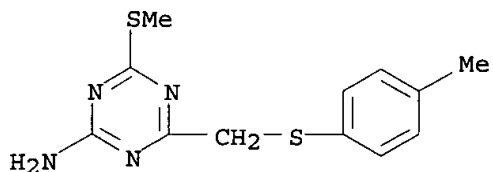


=> d l36 REF

L36 ANSWER 1 OF 5 CHEMCATS COPYRIGHT 2002 ACS
 Accession No. (AN): 1998:635165 CHEMCATS

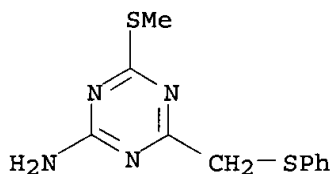
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L36 ANSWER 1 OF 5 CHEMCATS COPYRIGHT 2002 ACS
 Accession No. (AN): 1998:635165 CHEMCATS
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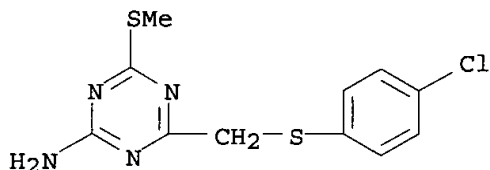


L36 ANSWER 2 OF 5 CHEMCATS COPYRIGHT 2002 ACS
 Accession No. (AN): 1998:635164 CHEMCATS
 Catalog Name (CO): Maybridge HTS
 Publication Date (PD): 6 Feb 2002
 Order Number (ON): SPB 06115

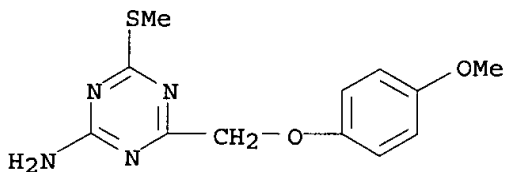
Chemical Name (CN): 4-(methylthio)-6-[(phenylthio)methyl]-1,3,5-triazin-2-amine
 CAS Registry No. (RN): 265314-65-6
 Supplementary Term (ST): CHEMICAL LIBRARY
 Structure :



L36 ANSWER 3 OF 5 CHEMCATS COPYRIGHT 2002 ACS
 Accession No. (AN): 1998:635163 CHEMCATS
 Catalog Name (CO): Maybridge HTS
 Publication Date (PD): 6 Feb 2002
 Order Number (ON): SPB 06114
 Chemical Name (CN): 4-[[[4-chlorophenyl]thio]methyl]-6-(methylthio)-1,3,5-triazin-2-amine
 CAS Registry No. (RN): 265314-64-5
 Supplementary Term (ST): CHEMICAL LIBRARY
 Structure :



L36 ANSWER 4 OF 5 CHEMCATS COPYRIGHT 2002 ACS
 Accession No. (AN): 1998:634797 CHEMCATS
 Catalog Name (CO): Maybridge HTS
 Publication Date (PD): 6 Feb 2002
 Order Number (ON): SPB 05667
 Chemical Name (CN): 4-[[[4-methoxyphenoxy]methyl]-6-(methylthio)-1,3,5-triazin-2-amine
 CAS Registry No. (RN): 266679-33-8
 Supplementary Term (ST): CHEMICAL LIBRARY
 Structure :



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09/732,546

Accession No. (AN): 1998:634796 CHEMCATS
Catalog Name (CO): Maybridge HTS
Publication Date (PD): 6 Feb 2002
Order Number (ON): SPB 05666
Chemical Name (CN): 4-[(2-chlorophenoxy)methyl]-6-(methylthio)-1,3,5-triazin-2-amine
CAS Registry No. (RN): 266679-32-7
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :

